PB89-124358

# Kinetic Modeling of NOx Formation and Destruction and Combustibles Burnout

Energy and Environmental Research Corp.
Irvine, CA

Prepared for

Environmental Protection Agency
Research Triangle Park, NC

Oct 88

U.S. Department of Commerce
National Technical Information Service
NTIS

PB89-124358

EPA/600/7-88/021
October 1988

# KINETIC MODELING OF $NO_x$ FORMATION AND DESTRUCTION AND COMBUSTIBLES BURNOUT

by

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EPA Contract No. 68-02-4247, task 2

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## TECHNICAL REPORT DATA

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| | | |
|---|---|---|
| 1. REPORT NO.<br>EPA/600/7-88/021 | 2. | 3. RECIPIENT'S ACCESSION NO.<br>PB89 124356 |
| 4. TITLE AND SUBTITLE<br>Kinetic Modeling of NOx Formation and Destruction and Combustibles Burnout | | 5. REPORT DATE<br>October 1988 |
| | | 6. PERFORMING ORGANIZATION CODE |
| 7. AUTHOR(S)<br>J. A. Cole, J. C. Kramlich, and W. S. Lanier | | 8. PERFORMING ORGANIZATION REPORT NO. |
| 9. PERFORMING ORGANIZATION NAME AND ADDRESS<br>Energy and Environmental Research Corporation<br>18 Mason<br>Irvine, California 92718-2798 | | 10. PROGRAM ELEMENT NO. |
| | | 11. CONTRACT/GRANT NO.<br>68-02-4247, Task 2 |
| 12. SPONSORING AGENCY NAME AND ADDRESS<br>EPA, Office of Research and Development<br>Air and Energy Engineering Research Laboratory<br>Research Triangle Park, NC 27711 | | 13. TYPE OF REPORT AND PERIOD COVERED<br>Task Final; 10/85 - 8/88 |
| | | 14. SPONSORING AGENCY CODE<br>EPA/600/13 |

15. SUPPLEMENTARY NOTES AEERL project officer is William P. Linak, Mail Drop 65, 919/541-5792.

16. ABSTRACT The report describes a model of the gas-phase chemistry involved in the combustion of simple hydrocarbon fuels and the interconversion of fixed nitrogen species. One focus of the work was on modeling the chemistry involved in reburning and other advanced NOx control strategies. A second focus was on the decay rate of various hydrocarbon species under high-temperature conditions. This provided an initial step toward the chemistry needed to model fuel burnout in small combustors; e.g., wood stoves. The approach was to compare rates for elementary reactions as represented in the different compilations available in the literature. Where inconsistencies appeared, the original literature on the rates was consulted. The mechanism was tested against benchmark data so that the key reactions that controlled any inconsistencies could be identified. Adjustments to the rates were allowed if they fell within the error bounds of the original determination.

17. KEY WORDS AND DOCUMENT ANALYSIS

| a. DESCRIPTORS | b. IDENTIFIERS/OPEN ENDED TERMS | c. COSATI Field/Group |
|---|---|---|
| Pollution | Pollution Control | 13B |
| Nitrogen Oxides | Stationary Sources | 07B |
| Mathematical Models | | 12A |
| Kinetics | | 20K |
| Hydrocarbons | | 07C |
| Burnout | | 21B, 21H |

| | | |
|---|---|---|
| 18. DISTRIBUTION STATEMENT<br>Release to Public | 19. SECURITY CLASS *(This Report)*<br>Unclassified | 21. NO. OF PAGES<br>453 |
| | 20. SECURITY CLASS *(This page)*<br>Unclassified | 22. PRICE<br>[illegible] |

EPA Form 2220-1 (9-73)

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# ABSTRACT

The processes that govern $NO_x$ formation and fuel fragment burnout in practical combustion systems involve a tight coupling between gas-phase combustion chemistry, heat and mass transport, fluid dynamics, and heterogeneous reactions. Chemical reaction, however, accounts for all of the $NO_x$ formation and destruction that occurs in flames, as well as all fuel fragment burnout. Thus, the role of all the other processes is to set the environment against which the chemistry occurs. To adequately understand and predict $NO_x$ and fuel fragment behavior, some model of the chemistry is necessary.

A model of the gas-phase chemistry involved in the combustion of simple hydrocarbon fuels and the interconversion of fixed nitrogen species has been developed. A focus of the work was on modeling the chemistry involved in reburning and other advanced $NO_x$ control strategies. A second focus was on modeling the decay rate of various hydrocarbon species under high temperature conditions. This provided an initial step towards the chemistry needed to model fuel burnout in small combustors; e.g.,wood stoves.

The approach was to compare rates for elementary reactions as represented in the different compilations available in the literature. Where inconsistencies appeared, the original literature on the rates was consulted. The mechanism was tested against benchmark data, and the key reactions that controlled any inconsistencies were identified. Adjustments were allowed if they fell within the error bounds of the original determination.

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# LIST OF ABBREVIATIONS, SYMBOLS, AND TERMS

| Symbol | Meaning |
|---|---|
| A | Arrhenius pre-exponential factor, $cm^3$/mol/s |
| b | temperature exponent in modified Arrhenius expression, dimensionless |
| $E_a$ | Activation energy, cal/mol |
| K | Kelvins |
| $k_f$ | forward rate constant, $cm^3$-mol-s units |
| $k_r$ | reverse rate constant, $cm^3$-mol-s units |
| $\Delta H_f^{298}$ | enthalpy of formation from the elements at 298 K, kcal/mol |
| ppm | parts per million, gas volume basis |
| R | universal gas constant, 1.986 cal/mol/K |
| SR | stoichiometric ratio |
| t | time |
| T | temperature |
| TFN | total fixed nitrogen |

# ACKNOWLEDGEMENTS

The authors wish to acknowledge the many helpful suggestions made by R.K. Lyon. Professor C.T. Bowman of Stanford University also helped focus the evaluation of alternatives for several portions of the nitrogen mechanism.

# 1.0 INTRODUCTION

The control of oxides of nitrogen from practical sources has become a relatively mature science. This is not to say that scientific breakthroughs will not occur, for indeed they do. However, the basis for many of the proposed technologies are well understood on a qualitative bases. Thus, a major research thrust at the present time is developing the quantitative understanding necessary to optimize $NO_x$ control, and to aid in the design of scaled-up units.

A good example of such an $NO_x$ control technology is reburning. Over the last several years, a diagram showing the key reactions that govern the reburning process would have changed only in its minor details. However, calculations of reburning would have changed considerably because the kinetic rates associated with many of the key reactions have evolved over the same time frame.

This report covers the development of a chemical kinetic mechanism for $NO_x$ formation and destruction, and fuel fragment burnout. The goal of this development is to provide a state-of-the-art tool for the analysis, optimization, and generalization of these technologies. In other words, the work reported here is designed to help convert our qualitative understanding of these processes into a more quantitative understanding.

The overall processes that govern $NO_x$ behavior and fuel-fragment burnout in practical devices are very complex. They involve a close coupling between chemistry and the various multiphase transport processes. The role of the transport processes is to provide the compositional and thermal environment against which the chemistry occurs. Thus, the chemistry can be decoupled from the other rate processes, developed separately, and at least conceptually combined into a complete model. At the same time, the chemistry represents a limit case that is worthy of study on its own, for it provides the limit of performance when all transport processes have been aligned to provide the ideal environment.

## 1.1 Background

The reburning process is a good example of the new $NO_x$ control technologies which have arisen over the past few years. Reburning evolved from the observations of Myerson (1957) and the work of Patry (1950) which showed that CH4 fragments may reduce NO at high temperatures under fuel-rich conditions. The concept of reburning was developed by Reed (1969) and by Wendt (1974) who along with C.V. Sternling and M.A. Matovich coined the phrase "reburning."

The overall reburning process can be divided conceptually into three zones as illustrated in Figure 1-1:

- Primary Zone: This main heat release zone normally accounts for approximately 80 to 90 percent of the total heat input to the system and is run fuel-lean. The level of $NO_x$ exiting the zone is defined to be the input to the reburning process. In addition, if sufficient residence time is not provided, unburned fuel fragments may leave this zone and enter the reburning zone.

- Reburning Zone: The reburning fuel (normally 10 to 20 percent of the total fuel input to the boiler) is injected downstream of the primary zone to create a fuel-rich, $NO_x$ reduction zone. Reactive nitrogen enters this zone from two sources:1) the primary NOx created in the main heat release zone, and 2) the fuel nitrogen in the reburning fuel. These reactive nitrogen species react with the hydrocarbon fragments formed during the partial oxidation of the reburning fuel, primarily CHi species, to produce intermediate species such as HCN and NH3. Additionally, some nitrogen is converted to N2 and some is retained as NO. If the reburning fuel is a solid such as coal, nitrogen may also leave this zone as char nitrogen.

- Burnout Zone: In this final zone, air is added to produce overall fuel-lean conditions and oxidize all remaining fuel fragments. The total fixed nitrogen species (TFN = $NO_x$ + NH3 + HCN + char nitrogen) will either be oxidized to $NO_x$ or reduced to molecular nitrogen.

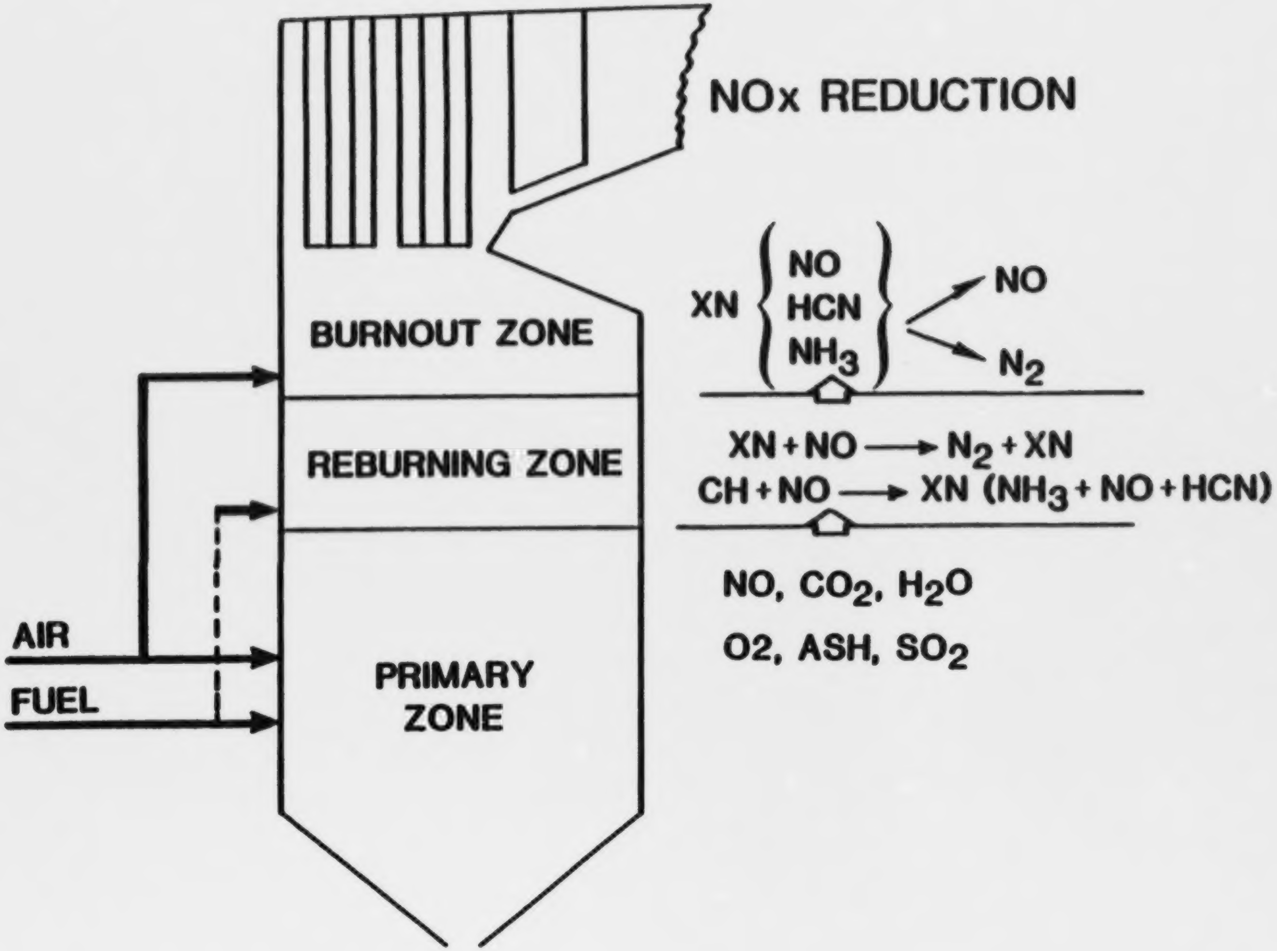
NOx REDUCTION
XN {NO HCN $NH_3$} → NO, $N_2$
BURNOUT ZONE
REBURNING ZONE
XN + NO → $N_2$ + XN
CH + NO → XN ($NH_3$ + NO + HCN)
PRIMARY ZONE
NO, $CO_2$, $H_2O$
O2, ASH, $SO_2$
AIR
FUEL

Figure 1-1. Schematic of the reburning process.

Experimental studies of reburning have raised many questions. Fuel type, reburning temperature and mixing configuration all impact the final $NO_x$ concentration. Also important are the primary and secondary (reburning) stoichiometries. Figure 1-2, for example, illustrates the impact of secondary zone stoichiometry on reburning in four experimental systems. Because of the many parametric studies of reburning and $NO_x$ reduction the overall understanding is fair. However, all of the key mechanisms are still not fully understood. Thus it is difficult to assign good values to all of the rate constants. Without this understanding, generalization is not possible and so far it has been difficult to predict even the trends in NOx reduction observed in laboratory and pilot-scale studies.

Equally as important to reburning is the hydrocarbon chemistry. Both during reburning fuel addition and during burnout, predicted $NO_x$ levels are sensitive to the details of hydrocarbon oxidation and hydrocarbon-nitrogen species interactions. During reburning fuel addition, $NO_x$ reduction depends upon the production and destruction of $CH_i$ fragments ($CH_3$, $CH_2$, CH). During burnout, the reactions responsible for oxidation of combustibles are also key to radical propagation. The balance of the radical pool species concentrations, as well as the rate of radical production, determine whether and how much of the residual fixed nitrogen is converted to $N_2$ and how much to NO.

In order to better understand and ultimately predict this process, a homogeneous kinetic mechanism was assembled. Currently the mechanism consists of the modified Arrhenius rate constants for 192 chemical reactions involving 40 species. It is solved with a model whose development and operation are described in a separate report (Kau 1987). The reburning process is ideally suited for homogeneous modeling because it is based on gas-phase reactions. Homogeneous models also lend themselves to simplicity in simulating a given environment.

## 1.2 Goals and Approach

The goals of this study are summarized as follows:

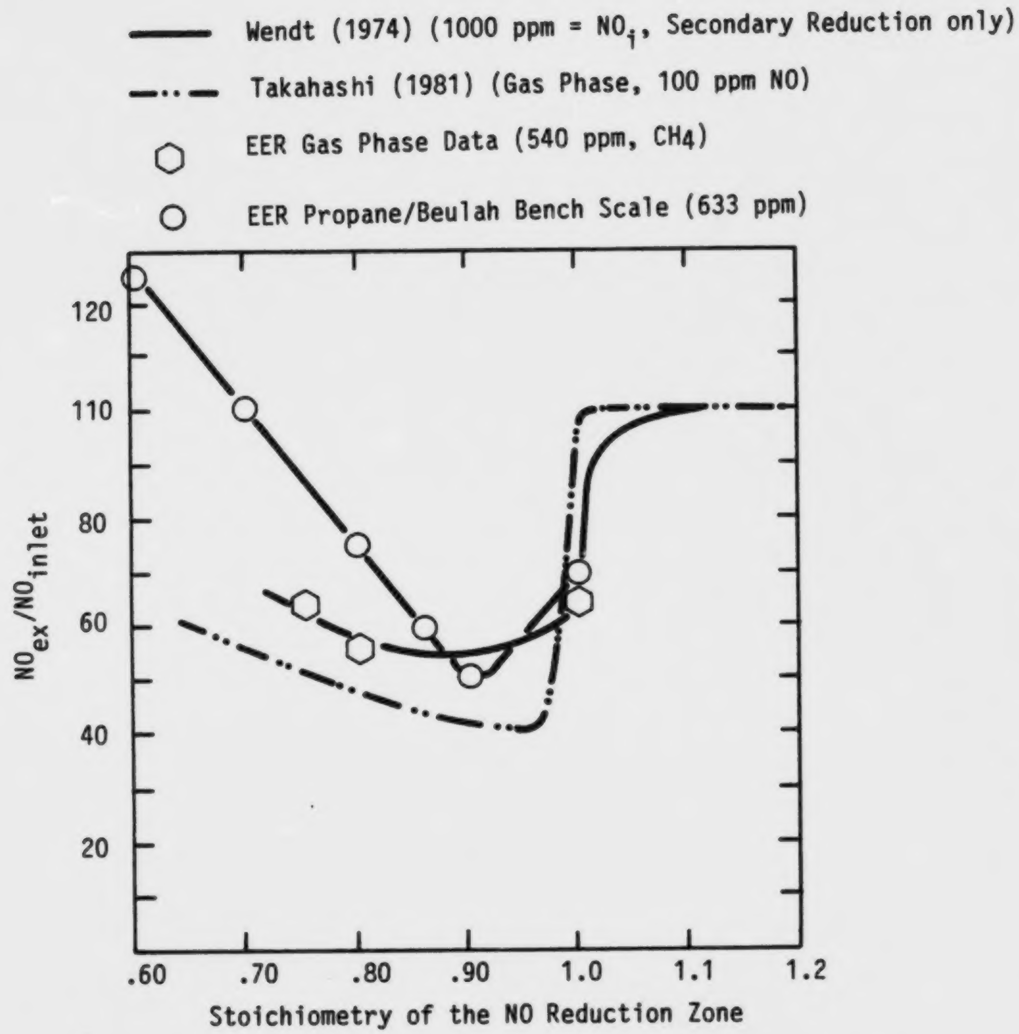

Figure 1-2. Effectiveness of reburning comparison of subscale data.

1) Effective modeling of $NO_x$ formation/destruction, e.g. reburning
2) Identification of as-yet-unknown key processes controlling $NO_x$ formation/destruction in practical combustion systems
3) Optimization of reburning in practical systems

The approach to these goals takes the following form:

1) Assemble an up-to-date homogeneous gas-phase kinetic mechanism for modeling combustion and nitrogen chemistry
2) Test the model against well characterized laboratory data
3) Identify specific areas for future improvements
4) Implement changes and incorporate new developments insofar as possible
5) Apply the mechanism to modeling the processes of interest e.g. reburning

## 2.0 NUMERICAL TOOLS

### 2.1 One-Dimensional Flame Code

The principal modeling tool for kinetic analysis is the One-Dimensional Flame code, or ODF. The code is basically a one-dimensional kinetics integrator that was developed from a more general two-dimensional parabolic diffusion flame solver (Kau, 1987). As such, it will accomodate 50 chemical species and 200 reactions in its present form. The algorithm is configured into a fully implicit form for high numerical stability, and is cast into a tri-diagonal matrix solution form for high speed non-iterative solution. The basic code can be configured as either a well-stirred reactor or a plug-flow reactor. The key features for the present applications include:

- Capability of modeling a premixed flame as a small well-stirred reactor followed by a plug-flow reactor. The well-stirred reactor acts as an ignition source, and the code allows the reactor transition to occur automatically within a single run.

- The reactor can be adiabatic, isothermal, have an arbitrarily specified temperature history, or an arbitrarily specified heat loss rate. Because of the great sensitivity of reburning to the thermal environment, the capability of forcing an experimentally measured temperature profile onto a calculation is a key capability.

- Sidestreams can be added at arbitrary locations. The sidestreams can be added at varying rates (e.g. all at once, or spread over a finite reactor time). This is a key capability for modeling both reburning fuel and reburning air addition

- A reaction screening option allows display of both the rank and percent contribution of the five key reactions which are both forming and destroying a selected species at any point in the reactor. This is an important capability for defining the controlling reactions in any given situation.

- The program will accept rate data in the modified Arrhenius format, which allows accommodation of almost all of the rate data presently published.

## 2.2 Utility Programs

Rate constants were initially assembled according to:

- Chemical reaction
- Chemical elements in each reaction
- Reference for rate data
- Direction of reaction
- Valid temperature range of rate data (if provided)

All of the rate data were co-plotted in Arrhenius format to facilitate rate selection. Examples of these plots are shown and discussed below. This is followed by a description of the utility programs which were written and used to organize the rate data and create the Arrhenius plots. The plots and tabular rate data are contained in Appendix A.

Comparison of rate constants from the different references on Arrhenius plots had several advantages:

- It facilitated comparison of forward and reverse rate constants
- Rate constants obtained over different temperature intervals could be juxtaposed

- rate data with strikingly different Arrhenius parameters were often revealed to have similar Arrhenius behavior.

Figure 2-1 illustrates the rate constants for the reaction NH3 + H = NH2 + H2. In this example widely different kinetic rates have been cited for the reaction. Although it is a simple metathesis reaction, a reliable direct measurement of the rate was not available until 1985 (Michael, 1985) and is cited by Glarborg (1986).

Figure 2-2 provides an example of a reaction whereof different rate data were obtained over several different temperature intervals. The juxtaposition of the curves in the figure suggest that a single modified Arrhenius expression might be in order to reconcile the data. Another feature of this figure is the similarity between the two rate constants cited by the Sandia group (Glarborg, 1985, 1986). The difference in the two rates amounts only to fine tuning of the mechanism, yet the similarity is not apparent in the rate expressions. Figure 2-3 illustrates an attempt to reconcile data obtained over different temperature intervals. Warnatz (1984) reviewed five sources of data and fitted them to an expression which accounts for the non-Arrhenius behavior of the reaction. Note also that the Warnatz expression is for the reverse rate constant. The expression chosen in this case is that provided by Glarborg (1986) which closely parallels the Warnatz value at reburning temperatures. The methodology for developing and using this tool follows.

In order to construct the plots, several FORTRAN programs were written on an IBM PC/AT and integrated with word processing and graphics software. One program was designed to organize all of the rate data according to the chemical reaction. This program then listed the rate constants along with the references and the valid temperature interval (if available, otherwise 1000-2000 K was used.) A second program calculated each reaction equilibrium constant and forward and reverse rate constants for each set of rate parameters over its valid temperature range. A third program selected the correct rate data, depending on whether the Arrhenius constants were given for the forward or reverse direction, and sent the information to a graphics printer.

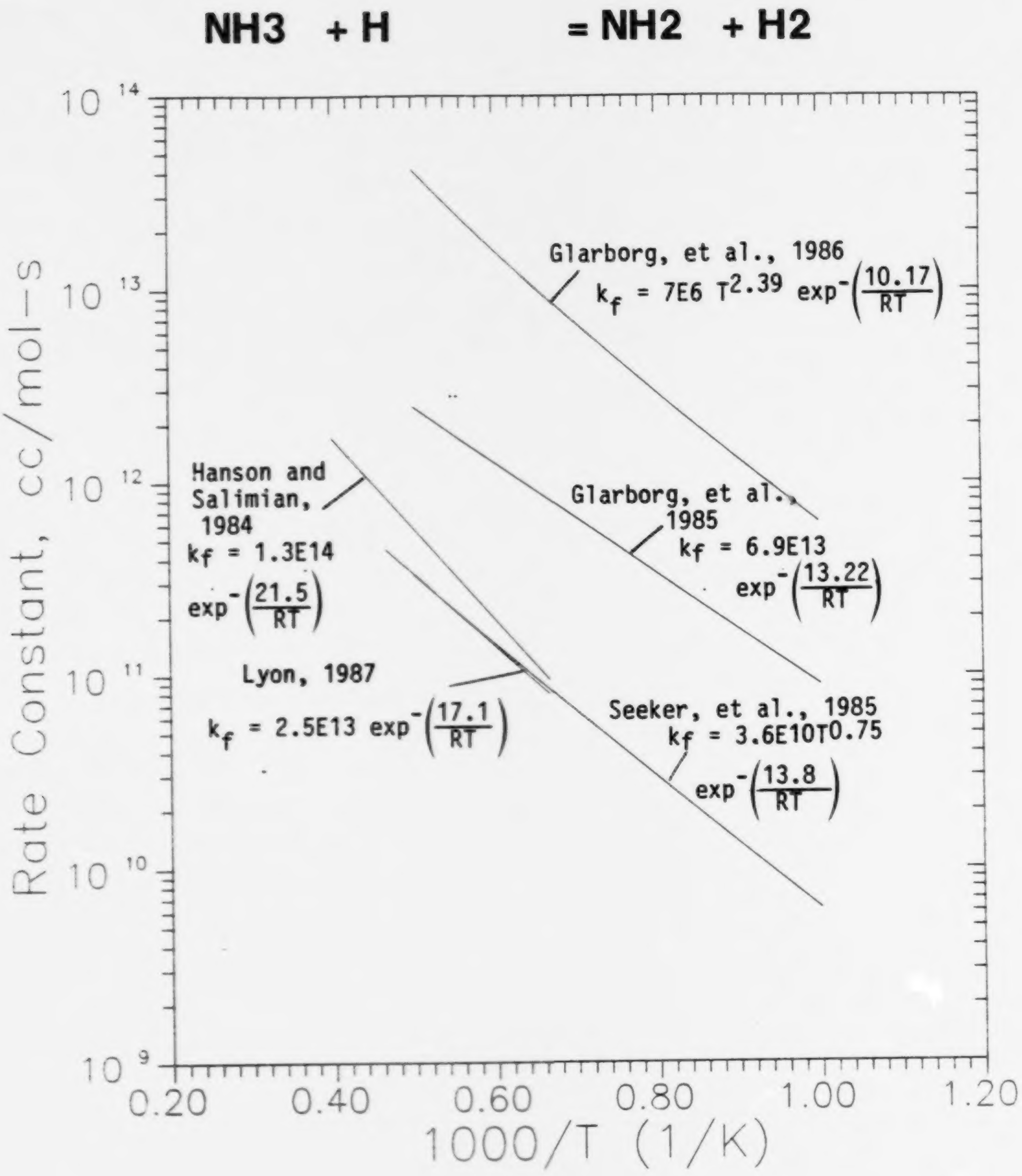

Figure 2-1. Rate constants for the reaction $NH_3 + H = NH_2 + H_2$

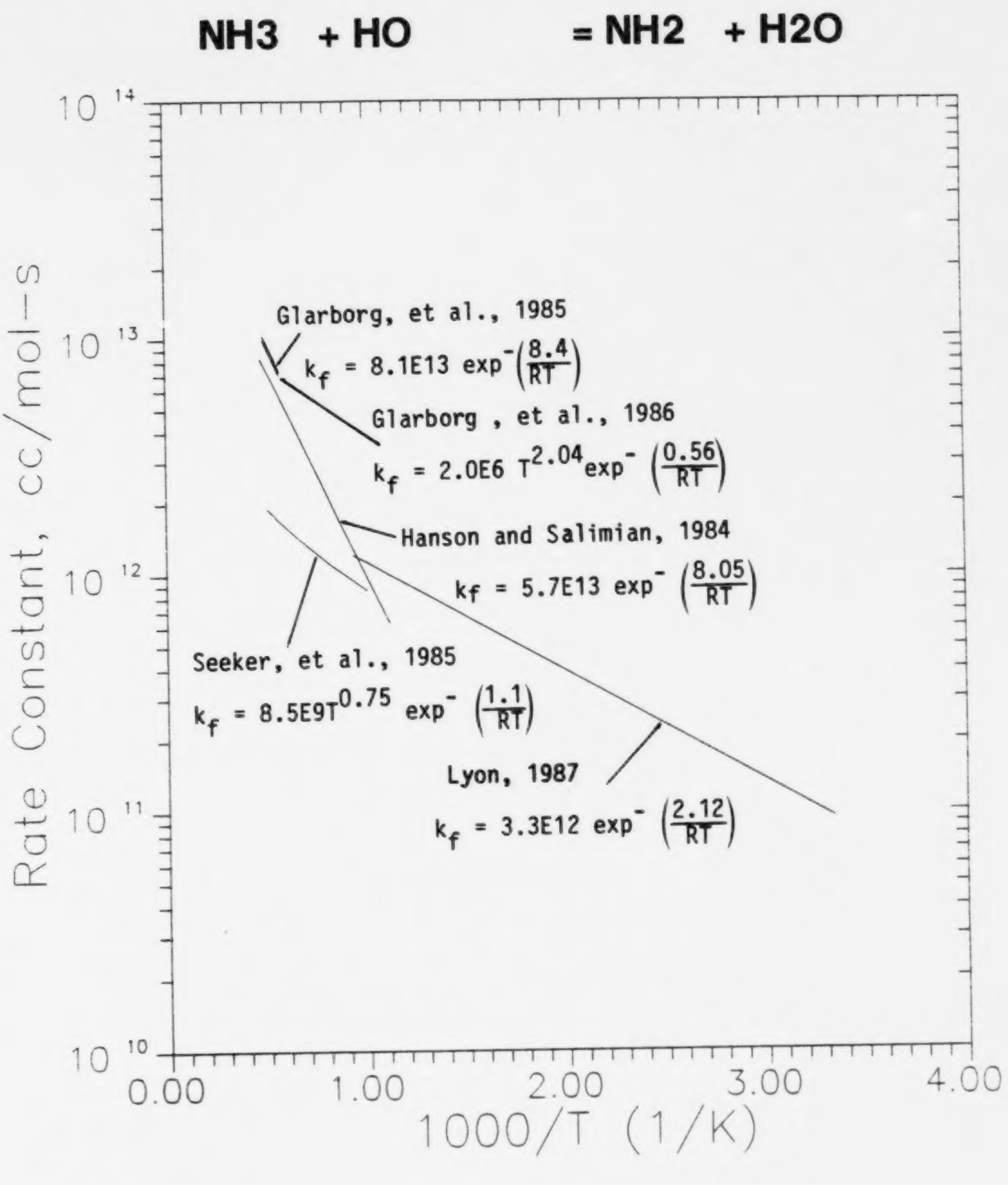

Figure 2-2. Rate constants for the reaction.
$NH_3 + HO = NH_2 + H_2O$

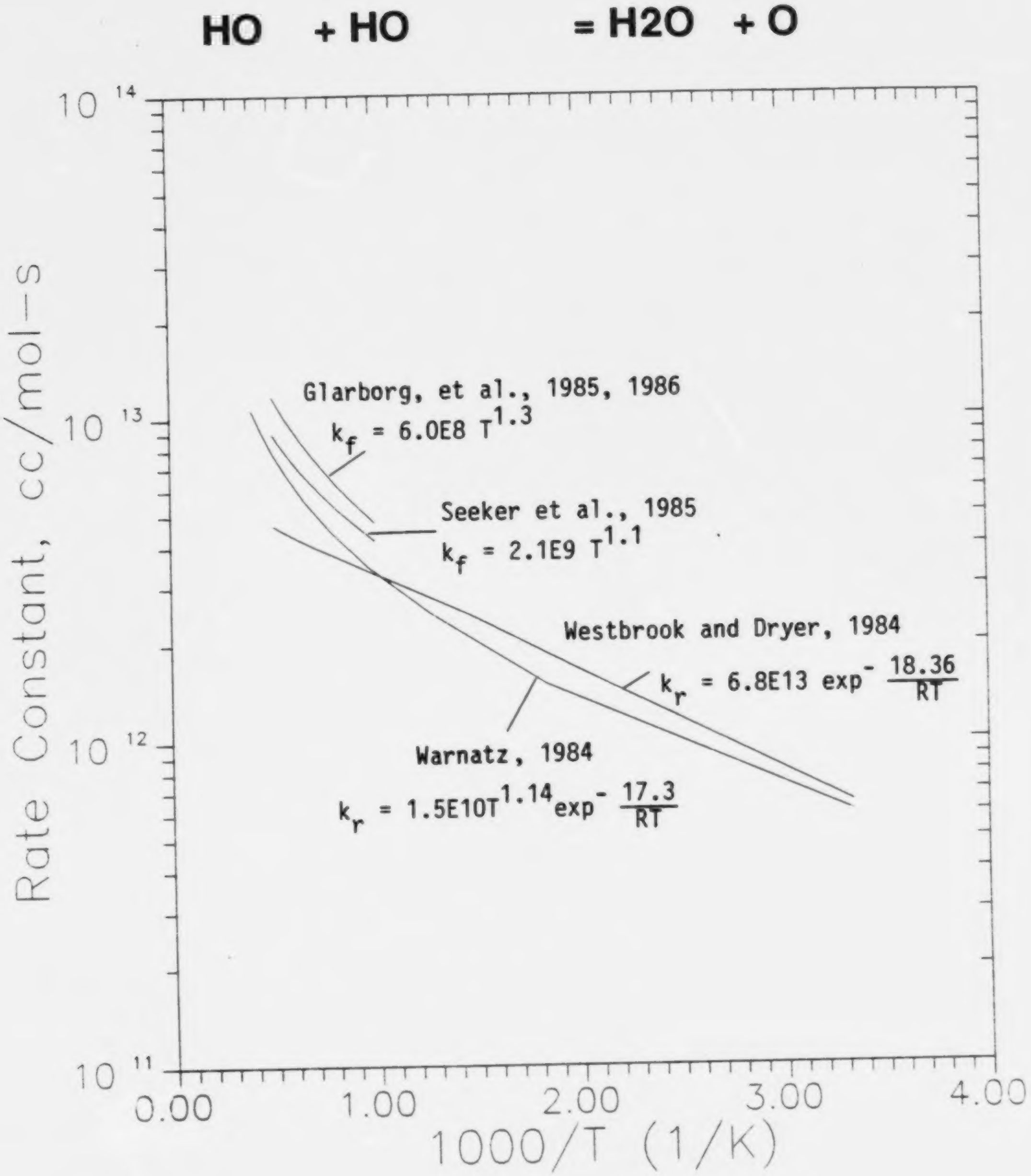

Figure 2-3. Rate constants for the reaction.
HO + HO = $H_2O$ + O

The first program accepted rate data typed in at the terminal and stored them along with the literature references in a formatted file. The program began by requesting the names for the reactants and products. It then requested the Arrhenius rate parameters and a valid temperature interval for the parameters (default = 1000-2000 K). Finally, the literature reference, or references, for the reactions were added and stored in an output file along with the above data.

A second program was used to read all of the individual reaction files and organize them into a table similar to that shown in Appendix A. For each reaction this table contained a rate expression, references, and the appropriate temperature interval. The table also indicated whither the rate expression was intended for the forward or reverse direction of the reaction as written.

Finally, a set of small programs was written to interface with the GRAPHER software package provided by Golden Graphics Co. These programs were controlled by a .BAT file. The programs would read from a set of rate data the rate expressions for a single reaction. After determining whether the data were for the forward or reverse directions, two tables were calculated. The first table contained 10 values for the forward rate constant over the indicated valid temperature interval.. The second table contained the corresponding values for the reverse direction.

After all of the rate data for a given reaction were so processed, the graphic program was called to create PLOT, and GRAPH files for the reaction. The PLOT and GRAPH files were first sent to a backup floppy disk, and then to a laser printer. This produced the Arrhenius plots shown in the Appendix. The process was repeated until the end of the reaction file was detected.

## 3.0 MECHANISM DEVELOPMENT

### 3.1 Methodology

A thorough search of the primary literature for kinetic rate data was beyond the scope of this program. It also was not considered to be the best use of the available resources. Many highly regarded researchers are specialists in evaluation of chemical kinetic data. Therefore, their work was used as reference in order to assemble a specialized mechanism.

Eight existing compilations and critical evaluations of kinetic rates were used as the principal sources for this study. These eight principal references are listed below.

1. Seeker (1985)
2. Lyon (1987)
3. Westbrook (1984)
4. Glarborg (1985)
5. Glarborg (1986)
6. Warnatz (1984)
7. Hanson (1984)
8. Tsang (1986)

The report by Seeker (1985) contains the current EPA mechanism developed under the FCR-I program. The FCR-I mechanism provided the starting point for the present mechanism development.

The global mechanism was divided into ten subsets according to the atomic species involved in each reaction (excluding chaperones.) These ten subsets are:

1. H2O2
2. CO
3. CH
4. CHO
5. NO
6. NH
7. NHO

8. HCN
9. NCO
10. HNCO

Each subset was developed separately. Once assembled the comprehensive mechanism consisted of 252 reactions of 46 species containing up to three carbon atoms.

Preferred rates were selected according to several criteria. These were:

1. Evaluation of rate expressions. e.g. is the expression reasonable for that type of reaction?
2. Original source of rate constants. Was the rate measured, estimated, or inferred?
3. Experimental technique used to obtain rate data.
4. Temperature range of the rate measurement.
5. Discussion by authors of cited references.
6. Freshness of the data.
7. Proximity of Arrhenius curve to others for same reaction. i.e. is the data a reasonable fit to disparate measured values?

When these factors were considered the "best" rate data were usually obvious. For many reactions, however, the differences between rate expressions were negligible and so the choice became immaterial. The latter observation prevailed in the H2O2 subset where rate data are relatively accurate for most reactions.

The most difficult data to evaluate are those which are in transition between their high- and low-pressure limits under reburning conditions. In general there is no simple expression which accurately describes the pressure dependence of these rates. Fortunately, the reburning process is currently limited to pressures near 1 atm and a relatively narrow temperature range. These restrictions simplified calculation of accurate modified Arrhenius parameters using available data.

A major concern in the development and implementation of a kinetic mechanism is the large number of species and reactions. If Occam's razor were strictly applied, every species and every mechanism which was not absolutely required should have to be eliminated. Of course, that would require a sensitivity analysis for each one under all possible conditions of interest. Fortunately, there is a less drastic approach which may be followed.

The key is to find, first of all, what species could be omitted without damaging the realism of the mechanism. There are several. Ozone is a significant species only at much lower temperatures than are of interest for reburning. $CH_3O$ and $CH_2OH$ probably don't interconvert, but their rate constants, where known, are quite similar and their thermodynamics are close. Thus, it is a reasonable approximation to eliminate one of them by writing all reactions in terms of the other. Reburning is concerned mainly with hydrocarbon fragments which are formed from methane and acetylene. Thus, it is possible to eliminate all species containing 3 or more carbon atoms without sacrificing too much realism for these conditions.

Secondly, many reactions were identified which either are no longer considered valid, or which are known as unimportant under reburning conditions. Examples are

$$O_2 + H_2 = OH + OH$$

which is a symmetry-forbidden four-center reaction, or

$$CH_2 + O_2 = CO_2 + H_2O$$

for which recent experiments (Hwang, 1987) find no evidence.

In all, 6 species and 60 reactions were eliminated to produce the present mechanism.

## 3.2 The Mechanism

The present kinetic mechanism is shown in Table I. It contains 192 reactions involving 40 species. The mechanism is divided into 10 subparts based on the atomic species contained in the reactants.

TABLE I. KINETIC REACTION MECHANISM

| | REACTION | | | | | | | Rate Constants** | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | A | b | Ea | footnotes |
| 1 | H | + O2 | | = | HO | + O | | 5.10E+16 | 0.82 | 16500 | a,b |
| 2 | H2 | + O | | = | HO | + H | | 1.80E+10 | -1.0 | 8800 | a,b,c,d |
| 3 | H2 | + HO | | = | H2O | + H | | 1.20E+09 | -1.3 | 3600 | a,b |
| 4 | H | + H | + M | = | H2 | + M | | 1.00E+18 | 1.0 | 0 | a |
| 5 | H | + H | + H2 | = | H2 | + H2 | | 9.70E+16 | 0.6 | 0 | e |
| 6 | H | + H | + H2O | = | H2 | + H2O | | 6.00E+19 | 1.2 | 0 | e |
| 7 | H | + H | + CO2 | = | H2 | + CO2 | | 5.50E+20 | 2.0 | 0 | e |
| 8 | H | + O2 | + M | = | HO2 | + M | | 2.10E+18 | 1.0 | 0 | a,b |
| 9 | HO | + HO | | = | H2O | + O | | 6.00E+08 | -1.3 | 0 | a,b |
| 10 | HO | + H | + M | = | H2O | + M | | 7.50E+23 | 2.6 | 0 | a |
| 11 | HO2 | + H | | = | H2 | + O2 | | 2.50E+13 | 0.0 | 700 | a,b,c,d,e |
| 12 | HO2 | + H | | = | HO | + HO | | 2.50E+14 | 0.0 | 1900 | a,b,c,d |
| 13 | HO2 | + H | | = | H2O | + O | | 5.00E+13 | 0.0 | 1000 | d |
| 14 | HO2 | + O | | = | HO | + O2 | | 4.80E+13 | 0.0 | 1000 | a,b |
| 15 | HO2 | + HO | | = | H2O | + O2 | | 5.00E+13 | 0.0 | 1000 | a,b,c,d |
| 16 | HO2 | + HO2 | | = | H2O2 | + O2 | | 2.00E+12 | 0.0 | 0 | a,b,d,e |
| 17 | H2O2 | + M | | = | HO | + HO | + M | 1.29E+33 | 4.86 | 53200 | j |
| 18 | H2O2 | + H | | = | HO2 | + H2 | | 1.70E+12 | 0.0 | 3700 | a,b,c,d |
| 19 | H2O2 | + H | | = | H2O | + HO | | 3.20E+14 | 0.0 | 8900 | d |
| 20 | H2O2 | + HO | | = | H2O | + HO2 | | 1.00E+13 | 0.0 | 1800 | a,b,d |
| 21 | O2 | + M | | = | O | + O | + M | 1.90E+11 | -0.5 | 95600 | a,b |
| 22 | O | + H | + M | = | HO | + M | | 1.00E+16 | 0.0 | 0 | d |
| 23 | O | + HO | + M | = | HO2 | + M | | 1.00E+17 | 0.0 | 0 | d |
| 24 | CO | + O | + M | = | CO2 | + M | | 2.36E+15 | 0.0 | 4340 | f |
| 25 | CO | + O2 | | = | CO2 | + O | | 2.50E+12 | 0.0 | 47700 | a,b,d,e,f |
| 26 | CH4 | + M | | = | CH3 | + H | + M | 2.00E+17 | 0.0 | 88000 | d,e |
| 27 | CH4 | + H | | = | CH3 | + H2 | | 2.20E+04 | -3.0 | 8700 | a,b,d,e |
| 28 | CH4 | + CH2 | | = | CH3 | + CH3 | | 1.30E+13 | 0.0 | 9500 | a |
| 29 | CH4 | + CH | | = | C2H4 | + H | | 6.00E+13 | 0.0 | 0 | a,b |
| 30 | CH3 | + CH3 | + M | = | C2H6 | + M | | 1.87E+32 | 4.74 | 0 | j |
| 31 | C2H5 | + H | | = | CH3 | + CH3 | | 3.00E+13 | 0.0 | 0 | e |
| 32 | CH3 | + CH3 | | = | C2H4 | + H2 | | 2.10E+14 | 0.0 | 19200 | a,b |

### TABLE I. KINETIC REACTION M MECHANISM (cont'd)

| | REACTION | | | | Rate Constants** | | | |
|---|---|---|---|---|---|---|---|---|
| | | | | | A | b | Ea | footnotes |
| 33 | CH3 + M | = | CH2 + H | + M | 1.00E+16 | 0.0 | 90600 | e |
| 34 | CH3 + H | = | CH2 + H2 | | 9.00E+13 | 0.0 | 15100 | a,b |
| 35 | CH3 + CH2 | = | C2H4 + H | | 4.00E+13 | 0.0 | 0 | e |
| 36 | CH3 + CH | = | C2H3 + H | | 3.00E+13 | 0.0 | 0 | a,b |
| 37 | CH3 + C | = | C2H2 + H | | 5.00E+13 | 0.0 | 0 | a,b |
| 38 | CH2 + C2H6 | = | C2H5 + CH3 | | 2.20E+13 | 0.0 | 8700 | a |
| 39 | CH2 + C2H3 | = | C2H2 + CH3 | | 3.00E+13 | 0.0 | 0 | a,b,d |
| 40 | CH2 + H | = | CH + H2 | | 6.19E+17 | 1.45 | 0 | j |
| 41 | CH2 + CH | = | C2H2 + H | | 4.00E+13 | 0.0 | 0 | a,b |
| 42 | CH2 + CH2 | = | C2H2 + H2 | | 3.20E+13 | 0.0 | 0 | a,b,c,d,f |
| 43 | CH2 + CH2 | = | C2H3 + H | | 5.00E+12 | 0.0 | 0 | d |
| 44 | CH2 + C | = | C2H + H | | 5.00E+13 | 0.0 | 0 | a,b |
| 45 | CH + H | = | C + H2 | | 5.00E+13 | 0.0 | 0 | a,b |
| 46 | C2H6 + H | = | C2H5 + H2 | | 5.40E+02 | -3.5 | 5200 | a,b,c,d,e |
| 47 | C2H5 + M | = | C2H4 + H | + M | 4.11E+39 | 7.05 | 39700 | j |
| 48 | C2H4 + M | = | C2H2 + H2 | + M | 2.60E+17 | 0.0 | 79300 | a,c |
| 49 | C2H4 + H | = | C2H3 + H2 | | 1.50E+07 | -2.0 | 6000 | d |
| 50 | C2H3 + M | = | C2H2 + H | + M | 3.06E+44 | 8.25 | 49600 | j |
| 51 | C2H3 + H | = | C2H2 + H2 | | 2.00E+13 | 0.0 | 0 | e |
| 52 | C2H3 + C2H | = | C2H2 + C2H2 | | 3.00E+13 | 0.0 | 0 | a,b,d |
| 53 | C2H2 + M | = | C2H + H | + M | 4.00E+16 | 0.0 | 107000 | e |
| 54 | C2H + H2 | = | C2H2 + H | | 4.10E+06 | -2.4 | 900 | a,b,d |
| 55 | CH4 + O2 | = | CH3 + HO2 | | 7.90E+13 | 0.0 | 56000 | d |
| 56 | CH4 + HO | = | CH3 + H2O | | 3.50E+03 | -3.1 | 2000 | a,b,d |
| 57 | CH4 + HO2 | = | CH3 + H2O2 | | 2.00E+13 | 0.0 | 18000 | c,d |
| 58 | CH3 + O2 | = | CH3O + O | | 7.00E+12 | 0.0 | 25700 | a,b,c,d,e |
| 59 | CH4 + O | = | CH3 + HO | | 1.20E+07 | -2.1 | 7600 | a,b |
| 60 | CH3 + O | = | CH2O + H | | 7.00E+13 | 0.0 | 0 | f,j |
| 61 | CH3 + HO | = | CH3O + H | | 5.40E+13 | 0.0 | 0 | f,j |
| 62 | CH3 + HO | = | CH2 + H2O | | 1.50E+13 | 0.0 | 5000 | a |
| 63 | CH3 + HO2 | = | CH3O + HO | | 2.00E+13 | 0.0 | 5000 | d |

TABLE I. KINETIC REACTION MECHANISM (cont'd)

| REACTION | Rate Constants** | | | |
|---|---|---|---|---|
| | A | b | Ea | footnotes |
| 64 CH3 + CH2O = CHO + CH4 | 1.00E+10 | -0.5 | 6000 | d |
| 65 CH3 + CHO = CO + CH4 | 3.00E+11 | -0.5 | 0 | d |
| 66 CH2 + O2 = CO + H2O | 3.90E+12 | 0.0 | 1400 | g,j |
| 67 CH2 + O2 = CO + HO + H | 9.10E+12 | 0.0 | 1400 | g,j |
| 68 CH2 + O = CO + H + H | 3.00E+13 | 0.0 | 0 | a,b |
| 69 CH2 + O = CO + H2 | 5.00E+13 | 0.0 | 0 | a,b |
| 70 CH2 + HO = CH2O + H | 3.00E+13 | 0.0 | 0 | a |
| 71 CH2 + HO = CH + H2O | 4.50E+13 | 0.0 | 3000 | a |
| 72 CH2 + CO2 = CO + CH2O | 1.10E+11 | 0.0 | 1000 | a,b |
| 73 CH + O = CO + H | 4.00E+13 | 0.0 | 0 | e |
| 74 CH + HO = CHO + H | 3.00E+13 | 0.0 | 0 | a,b |
| 75 CH + O2 = CO + HO | 2.00E+13 | 0.0 | 0 | c,e |
| 76 CH + CO2 = CHO + CO | 3.40E+12 | 0.0 | 700 | a,b |
| 77 C2H6 + O = C2H5 + HO | 3.00E+07 | -2.0 | 5100 | e |
| 78 C2H6 + HO = C2H5 + H2O | 6.30E+06 | -2.0 | 600 | e |
| 79 C2H6 + O2 = C2H5 + HO2 | 1.00E+13 | 0.0 | 51000 | d |
| 80 C2H5 + O2 = C2H4 + HO2 | 2.00E+12 | 0.0 | 5000 | e |
| 81 C2H5 + O = CH2O + CH3 | 5.00E+13 | 0.0 | 0 | e |
| 82 C2H4 + HO = C2H3 + H2O | 6.30E+12 | 0.0 | 1200 | a,d |
| 83 C2H4 + HO = CH2O + CH3 | 2.00E+12 | 0.0 | 1000 | a,b,d |
| 84 C2H4 + O = CHO + CH3 | 1.60E+09 | -1.2 | 700 | a,b,e |
| 85 C2H4 + O = CH2O + CH2 | 2.50E+13 | 0.0 | 5000 | d |
| 86 C2H3 + O2 = C2H2 + HO2 | 1.00E+12 | 0.0 | 10000 | d |
| 87 C2H3 + HO = C2H2 + H2O | 5.00E+12 | 0.0 | 0 | a,b,d |
| 88 C2H2 + O2 = CHO + CHO | 4.00E+12 | 0.0 | 28000 | c,d |
| 89 C2H2 + O = CH2 + CO | 4.10E+08 | -1.5 | 1700 | e |
| 90 C2H2 + HO = C2H + H2O | 6.30E+12 | 0.0 | 7000 | a,d |
| 91 C2H + O = CH + CO | 5.00E+13 | 0.0 | 0 | a,d,e |
| 92 C2H + O2 = CHO + CO | 2.40E+12 | 0.0 | 0 | a |
| 93 CH3O + M = CH2O + H + M | 1.00E+14 | 0.0 | 25000 | a,b,c,e |
| 94 CH3O + O = CH2O + HO | 1.00E+13 | 0.0 | 0 | a,b |
| 95 CH3O + O2 = CH2O + HO2 | 6.63E+10 | 0.0 | 2600 | a,b |

## TABLE I. KINETIC REACTION MECHANISM (cont'd)

| | Rate Constants** | | | |
|---|---|---|---|---|
| REACTION | A | b | Ea | footnotes |
| 96 CH3O + H = CH2O + H2 | 2.00E+13 | 0.0 | 0 | a,b,d,e |
| 97 CH3O + HO = CH2O + H2O | 1.00E+13 | 0.0 | 0 | a,b |
| 98 CH2O + M = CHO + H + M | 3.30E+16 | 0.0 | 81000 | a,b,c,d |
| 99 CH2O + O = CHO + HO | 3.50E+13 | 0.0 | 3500 | e |
| 100 CH2O + H = CHO + H2 | 2.20E+08 | -1.8 | 10500 | a |
| 101 CH2O + HO = CHO + H2O | 3.40E+09 | -1.2 | -400 | a |
| 102 CH2O +HO2 = CHO + H2O2 | 1.00E+12 | 0.0 | 8000 | c,d |
| 103 CHO + M = CO + H + M | 1.50E+14 | 0.0 | 14700 | a,c |
| 104 CHO + O2 = CO + HO2 | 5.12E+13 | 0.0 | 1690 | f |
| 105 CHO + O = CO + HO | 3.00E+13 | 0.0 | 0 | a,b,e |
| 106 CHO + O = CO2 + H | 3.00E+13 | 0.0 | 0 | a,b,e |
| 107 CHO + HO = CO + H2O | 3.00E+13 | 0.0 | 0 | f |
| 108 CHO + H = CO + H2 | 1.20E+14 | 0.0 | 0 | f |
| 109 CO + HO = CO2 + H | 5.47E+00 | -3.14 | -4970 | j |
| 110 CO + HO2 = CO2 + HO | 1.50E+14 | 0.0 | 23600 | e |
| 111 C + HO = CO + H | 5.00E+13 | 0.0 | 0 | a,b |
| 112 N + NO = N2 + O | 3.30E+12 | -0.3 | 0 | a,b |
| 113 N + O2 = NO + O | 6.40E+09 | -1.0 | 6300 | a,b,c |
| 114 NO2 + M = NO + O + M | 1.10E+16 | 0.0 | 66000 | a,b,h,i |
| 115 NO2 + O = NO + O2 | 1.00E+13 | 0.0 | 600 | a,b,c,h,i |
| 116 N2O + M = N2 + O + M | 1.60E+14 | 0.0 | 51600 | a,b |
| 117 N2O + O = NO + NO | 6.92E+13 | 0.0 | 26600 | h |
| 118 N2O + O = N2 + O2 | 1.00E+14 | 0.0 | 28200 | a,b,h |
| 119 NH3 + M = NH2 + H + M | 4.80E+16 | 0.0 | 93900 | i |
| 120 NH3 + H = NH2 + H2 | 7.00E+06 | -2.4 | 10200 | a |
| 121 NH2 + H = NH + H2 | 6.90E+13 | 0.0 | 3600 | c |
| 122 NH2 + HN2 = N2 + NH3 | 1.00E+13 | 0.0 | 0 | i |
| 123 NH2 + NH = N2H2 + H | 5.00E+13 | 0.0 | 0 | a,b |
| 124 NH2 + N = N2 + H + H | 7.20E+13 | 0.0 | 0 | a,b |
| 125 NH + N = N2 + H | 3.00E+13 | 0.0 | 0 | a,b |
| 126 NH + H = N + H2 | 3.00E+13 | 0.0 | 0 | a,b |

TABLE I. KINETIC REACTION MECHANISM (cont'd)

| REACTION | | | | | | | Rate Constants** | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | A | b | Ea | footnotes |
| 127 | NH | + NH | = | N2 | + H2 | | 3.60E+11 | -0.6 | 1900 | c |
| 128 | NH | + M | = | N | + H | + M | 3.20E+21 | 2.0 | 83400 | h |
| 129 | HN2 | + M | = | N2 | + H | + M | 2.00E+14 | 0.0 | 30000 | i |
| 130 | HN2 | + H | = | N2 | + H2 | | 3.70E+13 | 0.0 | 3000 | a,b |
| 131 | N2H2 | + M | = | HN2 | + H | + M | 5.00E+16 | 0.0 | 50000 | a,b |
| 132 | N2H2 | + H | = | HN2 | + H2 | | 5.00E+13 | 0.0 | 1000 | a,b |
| 133 | NH3 | + O | = | NH2 | + HO | | 2.10E+13 | 0.0 | 9000 | a,b |
| 134 | NH3 | + HO | = | NH2 | + H2O | | 3.30E+12 | 0.0 | 2100 | i |
| 135 | NH2 | + O | = | HNO | + H | | 6.60E+14 | 0.5 | 0 | a |
| 136 | NH2 | + O | = | NH | + HO | | 1.70E+13 | 0.0 | 1000 | i |
| 137 | NH2 | + NO | = | HN2 | + HO | | 6.10E+19 | 2.46 | 1870 | i |
| 138 | NH2 | + NO | = | N2 | + H2O | | 9.10E+19 | 2.46 | 1870 | i |
| 139 | NH2 | + O2 | = | HNO | + HO | | 5.10E+13 | 0.0 | 30000 | i |
| 140 | NH2 | + HO | = | NH | + H2O | | 5.50E+10 | -0.7 | 1300 | i |
| 141 | NH2 | + HNO | = | NH3 | + NO | | 1.80E+14 | 0.0 | 1000 | i |
| 142 | NH | + O2 | = | HNO | + O | | 1.00E+13 | 0.0 | 12000 | a,b |
| 143 | NH | + O2 | = | NO | + HO | | 1.40E+11 | 0.0 | 2000 | a,b |
| 144 | NH | + NO | = | N2O | + H | | 4.30E+14 | 0.5 | 0 | a,b |
| 145 | NH | + HO | = | HNO | + H | | 2.00E+13 | 0.0 | 0 | a,b |
| 146 | NH | + HO | = | N | + H2O | | 5.00E+11 | -0.5 | 2000 | a,b |
| 147 | N | + HO | = | NO | + H | | 3.80E+13 | 0.0 | 0 | a,b |
| 148 | HN2 | + HO | = | N2 | + H2O | | 3.00E+13 | 0.0 | 0 | h,i |
| 149 | HN2 | + NO | = | N2 | + HNO | | 9.10E+11 | 0.0 | 0 | i |
| 150 | NO | + HO2 | = | NO2 | + HO | | 3.40E+12 | 0.0 | -300 | i |
| 151 | NO2 | + H | = | NO | + HO | | 3.50E+14 | 0.0 | 1500 | a,b,h,i |
| 152 | N2O | + H | = | N2 | + HO | | 7.60E+13 | 0.0 | 15200 | a,b,c,h |
| 153 | HNO | + M | = | H | + NO | + M | 1.90E+16 | 0.0 | 48700 | i |
| 154 | HNO | + HO | = | NO | + H2O | | 3.60E+13 | 0.0 | 0 | a,b,i |
| 155 | HNO | + H | = | H2 | + NO | | 5.00E+12 | 0.0 | 0 | a,b |
| 156 | C | + NO | = | CN | + O | | 6.60E+13 | 0.0 | 0 | a |
| 157 | C | + N2O | = | CN | + NO | | 1.00E+13 | 0.0 | 0 | a,b |
| 158 | CN | + O | = | CO | + N | | 1.80E+13 | 0.0 | 0 | a,b |

TABLE I. KINETIC REACTION MECHANISM (cont'd)

|  | REACTION | Rate Constants** |  |  |  |
|---|---|---|---|---|---|
|  |  | A | b | Ea | footnotes |
| 159 | CN + O2 = NCO + O | 5.60E+12 | 0.0 | 0 | a,b |
| 160 | CN + NO2 = NCO + NO | 3.00E+13 | 0.0 | 0 | a,b |
| 161 | CN + N2O = NCO + N2 | 1.00E+13 | 0.0 | 0 | a,b |
| 162 | NCO + O = NO + CO | 5.60E+13 | 0.0 | 0 | a,b |
| 163 | NCO + N = N2 + CO | 2.00E+13 | 0.0 | 0 | a,b |
| 164 | NCO + M = N + CO + M | 3.10E+16 | 0.5 | 48000 | a,b |
| 165 | NCO + NO = N2O + CO | 1.00E+13 | 0.0 | -400 | a,b |
| 166 | N + CO2 = NO + CO | 1.90E+11 | 0.0 | 3400 | a,b |
| 167 | CH4 + N = NH + CH3 | 1.00E+13 | 0.0 | 24000 | a,b |
| 168 | CH4 + CN = CH3 + CHN | 3.20E+11 | -0.7 | 5000 | a |
| 169 | CH3 + N = CHN + H + H | 5.00E+13 | 0.0 | 0 | a,b |
| 170 | CH3 + CN = CH2 + CHN | 1.00E+11 | -0.7 | 3000 | a |
| 171 | CH2 + N2 = CHN + NH | 1.00E+13 | 0.0 | 74000 | a |
| 172 | CH2 + NH = CHN + H + H | 3.00E+13 | 0.0 | 0 | a,b |
| 173 | CH2 + N = CHN + H | 5.00E+13 | 0.0 | 0 | a,b |
| 174 | CH + N2 = CHN + N | 1.49E+12 | 0.0 | 13600 | j |
| 175 | CH + N = CN + H | 1.30E+13 | 0.0 | 0 | a |
| 176 | CH + NH2 = CHN + H + H | 3.00E+13 | 0.0 | 0 | a,b |
| 177 | CH + NH = CHN + H | 5.00E+13 | 0.0 | 0 | a,b |
| 178 | CN + H2 = CHN + H | 3.00E+05 | -2.5 | 2200 | a |
| 179 | CHN + HO = CN + H2O | 1.50E+13 | 0.0 | 10900 | a |
| 180 | CHN + HO = HNCO + H | 4.80E+11 | 0.0 | 11000 | a,b |
| 181 | CHN + HO = HOCN + H | 4.60E+12 | 0.0 | 15000 | j |
| 182 | CHN + O = NCO + H | 1.40E+04 | -2.6 | 5000 | a |
| 183 | CHN + O = NH + CO | 3.50E+03 | -2.6 | 5000 | a |
| 184 | CN + HO = NCO + H | 6.00E+13 | 0.0 | 0 | a |
| 185 | CH2 + NO = CHN + HO | 4.96E+12 | 0.0 | -1100 | j |
| 186 | CH + NO = CHN + O | 1.00E+14 | 0.0 | 0 | j |
| 187 | CH + NO = CHO + N | 1.00E+13 | 0.0 | 0 | j |
| 188 | NCO + H = NH + CO | 5.00E+13 | 0.0 | 0 | a,b |
| 189 | NCO + HO = NO + CO + H | 1.00E+13 | 0.0 | 0 | a,b |
| 190 | NCO + H2 = HNCO + H | 8.60E+12 | 0.0 | 9000 | a,b |

TABLE I. KINETIC REACTION MECHANISM (cont'd)

| REACTION | | | Rate Constants** A | b | Ea | footnotes |
|---|---|---|---|---|---|---|
| 191 HOCN + H | = | HNCO + H | 1.00E+13 | 0.0 | 0 | a |
| 192 HNCO + H | = | NH2 + CO | 2.00E+13 | 0.0 | 3000 | a,b |

chaperone efficiencies:

rxn 4: 0.000/H2 ; 0.000/H2O; 0.000/CO2

rxn 8: 3.300/H2 ;21.000/H2O; 5.000/CO2; 2.0/CO

rxn 10: 20.000/H2O

rxn 24: 1.525/CO2; 0.565/N2

rxn 26: 5.000/H2O

rxn 153: 2.000/H2 ; 2.000/O2 ; 6.000/H2O; 2.0/N2

footnotes:** k = A*(1/T)^b*exp(-Ea/RT) in cc-mol-s-cal units

a. Glarborg (1986)

b. Glarborg (1985)

c. Seeker (1985)

d. Westbrook (1984)

e. Warnatz (1984)

f. Tsang (1986)

g. Hwang (1987)

h. Hanson (1984)

i. Lyon (1987)

j see discussion in text

As the references in Table I suggest, the mechanism as a whole is essentially a modification of the Glarborg-Miller-Kee (GMK) mechanism (Glarborg, 1986). That, in turn, relied heavily upon the hydrocarbon oxidation mechanism of Westbrook and Dryer (Westbrook, 1984). The GMK mechanism was developed for the study of $NO_x$ formation in well-stirred reactors. Adapting the GMK mechanism to the rich-lean plug flow chemistry of reburning required many subtle changes which are discussed in detail below. However, the most apparent differences are the refinement of the fuel-rich hydrocarbon chemistry and the free radical pool chemistry using the recommendations of Warnatz (1984) and inclusion of the ammonia (thermal $DeNO_x$) chemistry of Lyon (1987).

The complete set of rate constants from which the mechanism was derived is provided in Appendix A. The tables in Appendix A also indicate the valid or measured temperature range (or default values) for each rate expression. Although the valid temperature range for many of the reactions was either unreported or did not cover the range for reburning, the rate expressions were used as provided except as discussed below.

The H2O2 mechanism (reactions 1-23) was largely taken from the compilations of Glarborg (1985, 1986). As the footnotes on the table suggest, there is generally a consensus among several authors concerning the rates in this mechanism. Even in the absence of absolute agreement, differences in the cited rate expressions tend to be small. This is illustrated in Figure 3-1 where four different Arrhenius expressions are compared on a single graph for reaction 3. In this case the largest disagreement is less than a factor of 2.

The CO mechanism, reactions 24 and 25 consists of only two reactions describing CO oxidation, while the CH mechanism, reactions 26-54, describes hydrocarbon pyrolysis and chain branching mechanisms. For reburning, only C1 and C2 species have been considered. Unimolecular decomposition of the four possible fuels is accounted for in reactions 26,30,48, and 53. Reaction 30 is also a key reaction in methane oxidation.

Hydrocarbon ignition and oxidation are described in the CHO mechanism (reactions 55-111). This is the largest subset in the reburning mechanism.

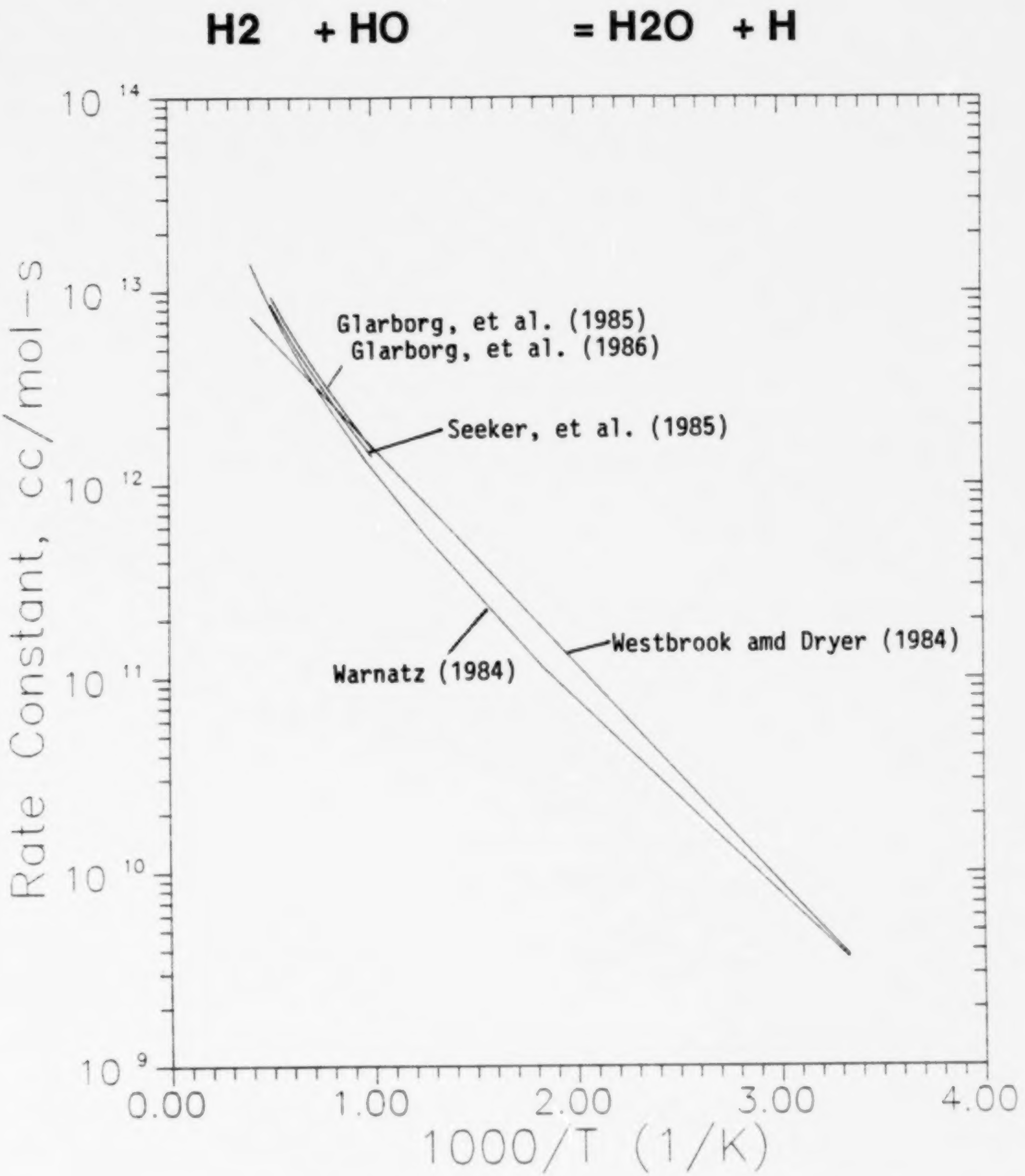

Figure 3-1. Comparison of rate constants provided by five authors for the reaction $H_2 + OH \rightleftharpoons H_2O + H$.

Most of the important chain branching and radical propagation steps are located here.

The NO, NH, and HNO mechanisms are provided in reactions 112-118, 119-132, and 133-155. These reactions concern ammonia oxidation and pyrolysis and the thermal deNOx mechanism. They are taken mainly from the compilations of Glarborg (1986) and Lyon (1987). The NCO (reactions 156-165) HCN (reactions 167-178) and HNCO (reactions 179-192) mechanisms contain the critical steps for reburning, NOx reduction, and HCN oxidation. The latter mechanisms were taken from Glarborg (1986) with the exception of reactions 186 and 187.

Several three-body reactions were identified as being in their fall-off regions at one atmosphere and at reburning temperatures. These are:

$H_2O_2 + M = HO + HO + M$ R17
$CH_3 + CH_3 + M = C_2H_6 + M$ R30
$C_2H_5 + M = C_2H_4 + H + M$ R47
$C_2H_3 + M = C_2H_2 + H + M$ R50

Rate constants for these reactions at one atmosphere over the temperature range of 1000-2500 K were obtained from Tsang (1986). Approximations to the rate curves were made using modified Arrhenius expressions. The rate expressions given in Table I provide accurate representations of the fall-off rates over the range of temperatures encountered during reburning.

Nitrogen fixation is strongly affected by the Fenimore reaction:

$CH + N_2 = CHN + N$ R174.

Glarborg (1986) chose a rate for R174 by adopting the activation energy of Matsui (1978) and then adjusting the pre-exponential factor so that the peak in their NO vs stoichiometry curve matched the data of Bartok (1972). We found that the rate of $N_2$-fixation was too slow using this rate. Therefore the preexponential factor inferred by Blawens (1977) was used along with the activation energy of Matsui (1978) to provide a rate approximately eight times as fast as Glarborg's. Even with the faster rate, however, the predicted levels of total fixed nitrogen (TFN) remained below the experimental values under fuel-rich conditions and were too high under fuel-lean conditions -- an observation which was also noted by Glarborg (1986) in a modeling study of NO formation in well-stirred reactors.

Reevaluation of Blawens' conclusions suggests that if R174 were indeed the sole source of prompt NO, then Blawens' rate should be a lower rather than an upper limit. This is because Blawens assumed that conversion of HCN to NO is 100 percent efficient. A sensitivity analysis of R174 showed that further increase in the preexponential produced an increase in predicted NO. This occurred as a result of the near collision rate reaction

N + O2 = NO + O R113.

The Fenimore reaction (R174) is also impacted by the assumed rate of CH formation. This is controlled by

CH2 + H = CH + H2 R40
CH2 + OH = CH + H2O R71
C2H + O = CH + CO R91

For R71 we have accepted the estimate of Glarborg(1986) which agrees well with the value obtained by Peeters (1975) at 2000 K. The rate for R91 was fairly well accepted by the cited references, although the value cited by Tsang (1986) was a bit lower (1.8E13 $cm^3$/mol·s) than the value cited here (5.0E13 $cm^3$/mol·s). This reaction is only important briefly during reburning: at the start of secondary fuel addition and during burnout, when the concentrations of both O-atom and ethynyl radical are significant.

The rate for R40 was obtained by accepting the room temperature value of Bohland (1984), as recommended by Tsang. This was then fitted to the shock-tube data of Frank (1984). A similar approach was also used by Glarborg (1986) although the value cited here is slightly higher at flame temperatures.

Direct reaction between oxygen and methylene has long been assumed to produce an array of products including CO, CO2, CHO and CH2O. Recently, however, Hwang (1987) has shown compelling evidence that CO2 is not formed directly through this addition. Rather, secondary routes such as

CO + OH = CO2 + H R109

are responsible for CO2 formation. The contrary reaction provides too high a heat release rate in the induction zone of acetylene flames. Following Hwang's recommendations we have included the reactions:

CH2 + O2 = CO + H2O R66
CH2 + O2 = CO + H + OH R67

with the rates k66 = 3.9E12 exp(-1400/RT) and k67 = 9.1E12 exp(-1400/RT). For the sake of consistency the formyl and formaldehyde routes have also been eliminated.

The rate for R109 was taken from Tsang (1986). His recommended expression is from Zellner (1979): k = 7.1E10 exp(0.00092xT). However, this form of rate expression cannot be accommodated by ODF. Therefore, the expression was fitted to the modified Arrhenius expression:

$$K109 = 5.466 * T^{3.14} exp(4970/RT).$$

This lies within five percent of the Zellner value over the temperature range of 1000-2500 K.

The rate of R181 was reduced to one-half of the value cited by Glarborg(1986) in order to improve the prediction of HCN and $NH_3$ production in the reburning zone.

Glarborg (1986) describes the reaction between $CH_2$ and NO by the sequence

$CH_2$ + NO = HCNO + H k = 1.4E12exp(+1100/RT)
HCNO + H = HCN + OH k = 5.0E13exp(-12000/RT)

The negative activation energy for the first step is reasonable because of the relatively stable adduct, $H_2CNO$ ( $H_f$ est. 36 kcal/mol) and high exothermicity (-78 kcal/mol) of the addition reaction. However, decomposition of nitrosomethylene into HCNO + H is 67 kcal endothermic. If this is followed by the slower attack of H-atom to finally produce HCN + OH then a substantial concentration of HCNO must accumulate. On the other hand, nitrosomethylene may decompose via unimolecular 1,3 H-shift for which an activation energy of only 40 kcal/mol (Benson, 1970) can be inferred. The resulting product - still in the excited state - will spontaneously decompose to HCN + OH with a net endothermicity of about 5 kcal/mol for the final step. Based upon the possibility of this alternative route, the products shown in R185 have been assumed. The rate constant was adjusted from Glarborg's value (for the addition reaction) to fit experimentally observed rates for NO disappearance after reburning fuel addition.

The reaction between $CH_3$ and O-atom, R60, leads to an excited methoxy radical. This may decompose by loss of either H-atom or $H_2$. Following the recommendation of Tsang (1986), the former has been incorporated into Table I. Methyl reaction with hydroxyl radical results in an excited $CH_3OH^*$ molecule. Spontaneous fission of the $CH_3OH^*$ to $CH_3O$ + H is in the fall-off region during reburning with approximately 50-70 percent of the $CH_3OH^*$ stabilized by collisions between 1000-1500 K. Since $CH_3OH$ has been omitted from the present mechanism, the overall rate recommended by Tsang (1986) was adopted and assigned to R61.

## 3.3 Reburning Chemistry

The chemistry controlling the reburning process is idealized in Figure 3-2. Elementary kinetics of higher hydrocarbon species are not shown on the figure. However, these complex hydrocarbons are destroyed during reaction, forming the simple hydrocarbons shown in the figure . Thusly they participate in the same chemistry. The key reactions are summarized below.

Acetylene appears as an intermediate during hydrocarbon oxidative pyrolysis. the major sink for C2H2 is:

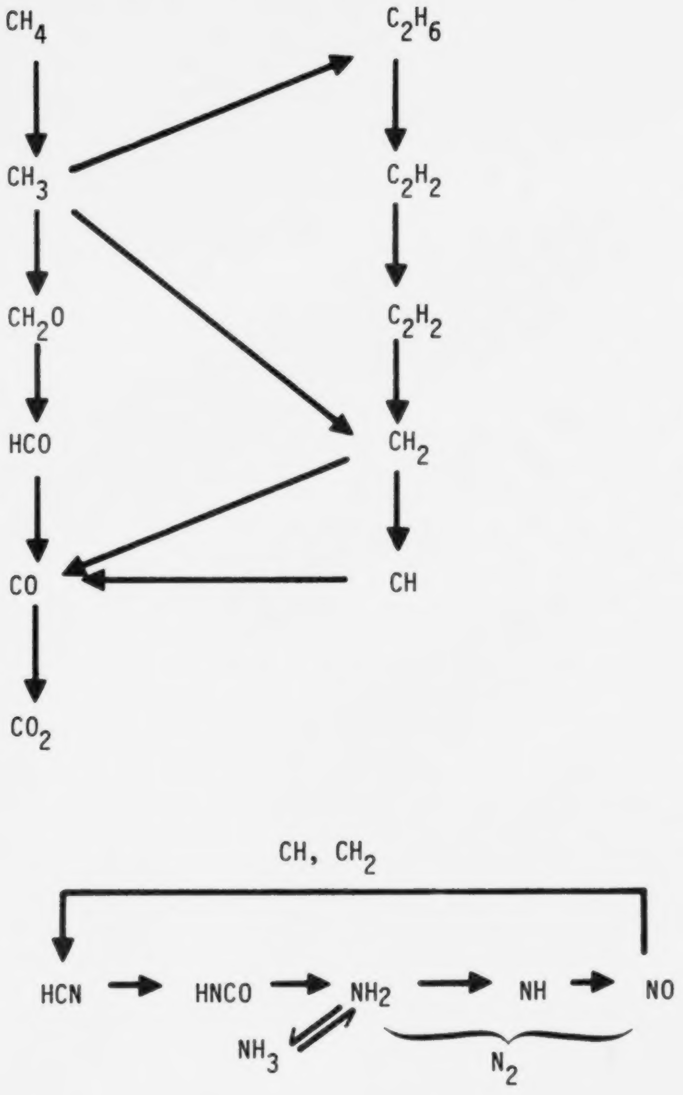
CH4
C2H6
CH3
C2H2
CH2O
C2H2
HCO
CH2
CO
CH
CO2
CH, CH2
HCN
HNCO
NH2
NH
NO
NH3
N2

Figure 3-2. Hydrocarbon and nitrogen chemistry relevant to reburning.

$C_2H_2 + O = CH_2 + CO.$ R89

This is also the principal source of CH2. The CH2 may react by either of two pathways:

$CH_2 + O_2 = CO + \text{products}$ R73, 74

$CH_2 + X = CH + XH.$

The CH and $CH_2$ radicals drive the bulk of the reburning process. Therefore, it is desirable that the CH formation reaction predominate over R73. The CH radical also has two competing sinks:

$CH + XO = \text{products}$

$CH + NO = \text{products}.$

Since it is the latter reaction which activates the reburning process, it is desirable to provide conditions which inhibit CH oxidation. One goal of modeling, therefore, is to identify conditions which minimize the oxidative reactions while maximizing the exposure of NO to CH and $CH_2$.

Much of the experimental effort in reburning has involved methane as the reburning fuel. This is mainly because of its low cost and ready availability compared with other hydrocarbon fuels (excluding N-containing fuels such as No.6 fuel oil). The chemistry of methane combustion is, therefore, central to understanding reburning. Despite the large body of work on the combustion of methane, the elementary processes involved are, at best, only poorly understood. One of the key steps in methane combustion is the removal of methyl radical. Westbrook and Dryer (1984) point to reaction 30

$CH_3 + CH_3 + M = C_2H_6 + M$ R30

as a critical sink for methyl radical, but also emphasize the importance of direct oxidation through

$CH_3 + O_2 = CH_3O + O.$ R58

The methoxy radical formed in reaction 58 has three major routes for destruction:

CH3O + M = CH2O + H + M R93
CH3O + O2 = CH2O + HO2 R95
CH3O + H = CH2O + H2. R96

Of these three reactions reaction 93 is most important during reburning. Reaction 95 is more important at low temperatures under very-fuel-lean stoichiometries while reaction 96 becomes significant at the start of both fuel and air staging, when the H-atom concentration rises dramatically.

Besides providing a route for methyl destruction reaction 58 is also an important chain branching step and provides a significant amount of H-atom.

Glarborg (1986) designates

CH + NO = CHN + O R186

as a "most important" reaction in NO formation in well-stirred reactors. Myerson (1975) however, argued on the basis of reaction coordinate energies that the alternate product distribution shown in reaction 187:

CH + NO = CHO + N R187

should also be significant. The resulting N-atom, according to Myerson, can then reduce NO through the reverse Zel'dovich mechanism:

N + NO = N2 + O. R112

When reaction 187 was added to the reburning mechanism it became the dominant source of N-atom which then drives reaction 112. The combined rate for reactions 186 and 187 was measured by Berman (1982) who found it to be 1.1E14 $cm^3$/mol/s, independent of temperature. The branching ratio assumed for these reactions is k186:k187 = 10:1 in the present mechanism. This value is not known, but may be considered adjustable although Glarborg (1986) concluded that reaction 186 is the most likely product channel.

## 4.0 MECHANISM VALIDATION AND TESTING

Validation of a kinetic model involves a comparison of the model's predictions with reliable data. An important consideration here is whether the experimental conditions can be accurately represented. Heat losses, wall effects, mixing and inhomogeneities all constitute modeling issues which go beyond chemical kinetics.

The present mechanism is first compared with shock-tube data. The tests were conducted following the format of an earlier study, the FCR-I program (Seeker, 1985), and the results are presented along with those of the latter. Secondly, the present mechanism is compared side-by-side with the FCR-I mechanism under simulated boiler reburning conditions. This comparison is divided into two parts. The first is a detailed look at the hydrocarbon combustion process, while the second examines differences in the way NOx reduction is effected in the two mechanisms.

### 4.1 Shock Tube Modeling

The hydrocarbon combustion mechanism was tested first following the procedure outlined in the FCR-I report by Seeker (1982). In this procedure the model is run in a shock tube format at one atmosphere. The ignition induction time is compared with experimental data. A shock tube is an ideal system for modeling because it is practically adiabatic, isobaric and isothermal. Seeker (1985) used an induction time defined as the time required for ten percent of the initial methane to be consumed. Following this approach a time parameter, B, was logarithmically correlated with inverse temperature. For the data of Seery and Bowman (1970) and the data of Skinner and Ruehrwein (1959)

$$B = t*(O2)^{1.6}*(CH4)^{-0.4}.$$

for the data of Grillo and Slack(1976) and Tsuboi and Wagner(1975)

$$B = t*(CH4)^{-0.32}*(O2)^{1.02}$$

where: t = induction time, s

(CH4) = CH4 concentration, $mol/cm^3$

(O2) = O2 concentration, $mol/cm^3$

Methane concentration trajectories are shown in Figure 4-1 for eight cases calculated using the present mechanism. Figures 4-2 through 4-4 show the results of the data correlations with the two mechanisms. The FCR-I mechanism (solid and broken lines) correlates best with the data in Figure 4-2. In Figures 4-3 and 4-4 the FCR-I mechanism predicts induction times faster than indicated by most of the data. The present mechanism (open crosses) predicts induction times somewhat slower than the data in Figure 4-2 but within the range of the data in Figures 4-3 and 4-4. Table II lists induction times predicted using the present mechanism.

## 4.2 Hydrocarbon Combustion Processes

The present mechanism was also compared with the FCR-I mechanism by running both under reburning conditions. The model was set up to simulate the chemistry and thermal history of the Hutsonville boiler of the Central Illinois Power Service Company. Coal firing was simulated by using acetylene at an initial stoichiometry of SR=1.1. The initial stoichiometry was reduced to SR=0.9 by a 10 ms addition of reburning fuel (CH4) at 1715 K. The behavior of the products of methane decomposition were then observed for each mechanism. Those species are of particular interest because of reactions 186 and 187 which are proposed as key to the reburning process.

Mole fraction profiles for the CHi species and O2 are shown in Figure 4-5 for the FCR-I mechanism and in Figure 4-6 for the present mechanism. Many features of the two plots are similar. In the 10 ms over which the CH4 is introduced the CHi species concentrations increase rapidly and the O2 concentration declines. The non-steady behavior of the $CH_i$ species profiles in this region is due to the delayed rise in flame radicals such as H, OH, O, and $HO_2$. These radicals begin to consume hydrocarbon fragments faster than $CH_4$ is being introduced, however they are abated as the O2 concentration declines.

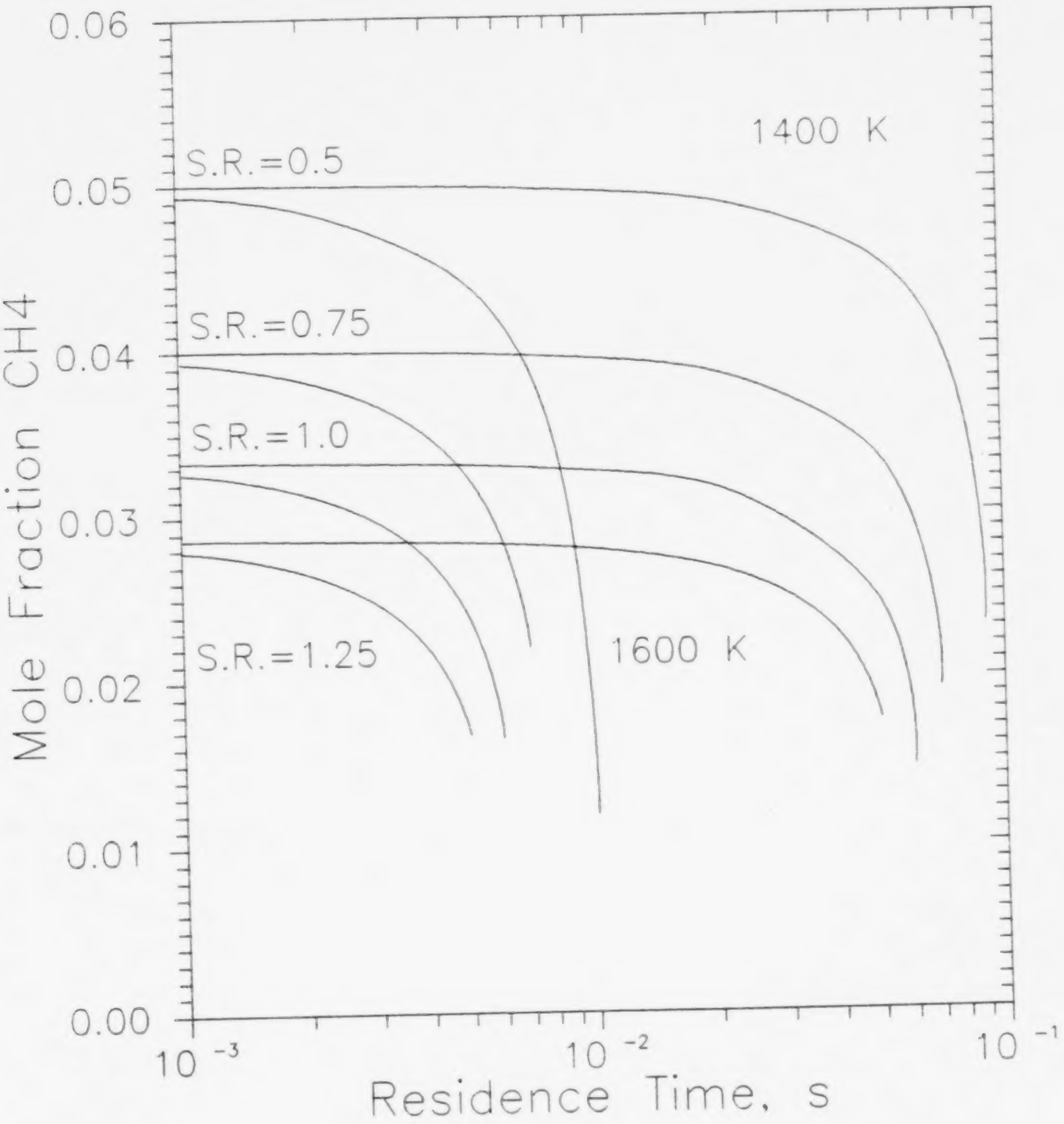

Figure 4-1. Shock-tube induction trajectories calculated using the FCR-III mechanism.

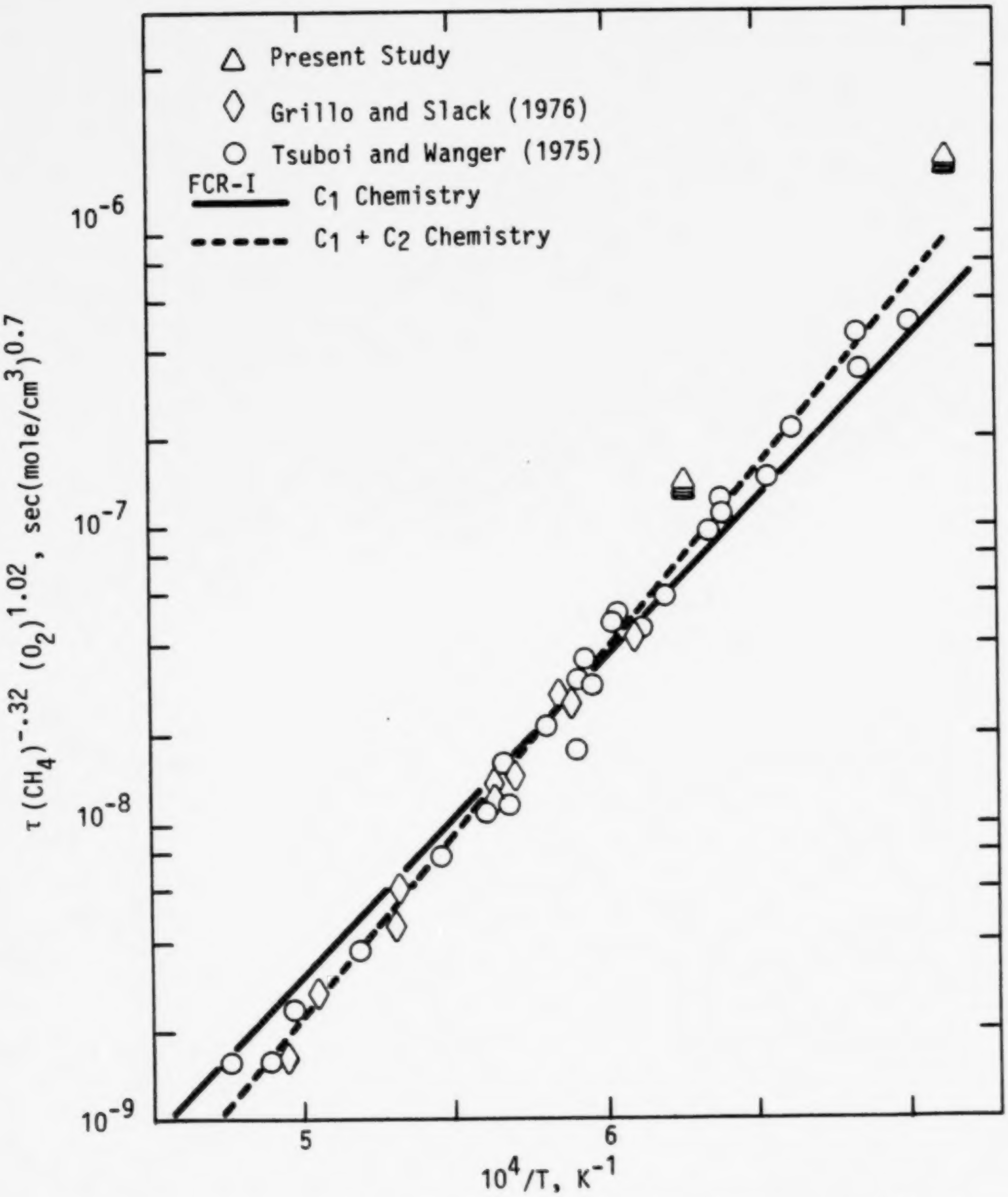

Figure 4-2. Correlation of $CH_4$-$O_2$-Ar induction times.

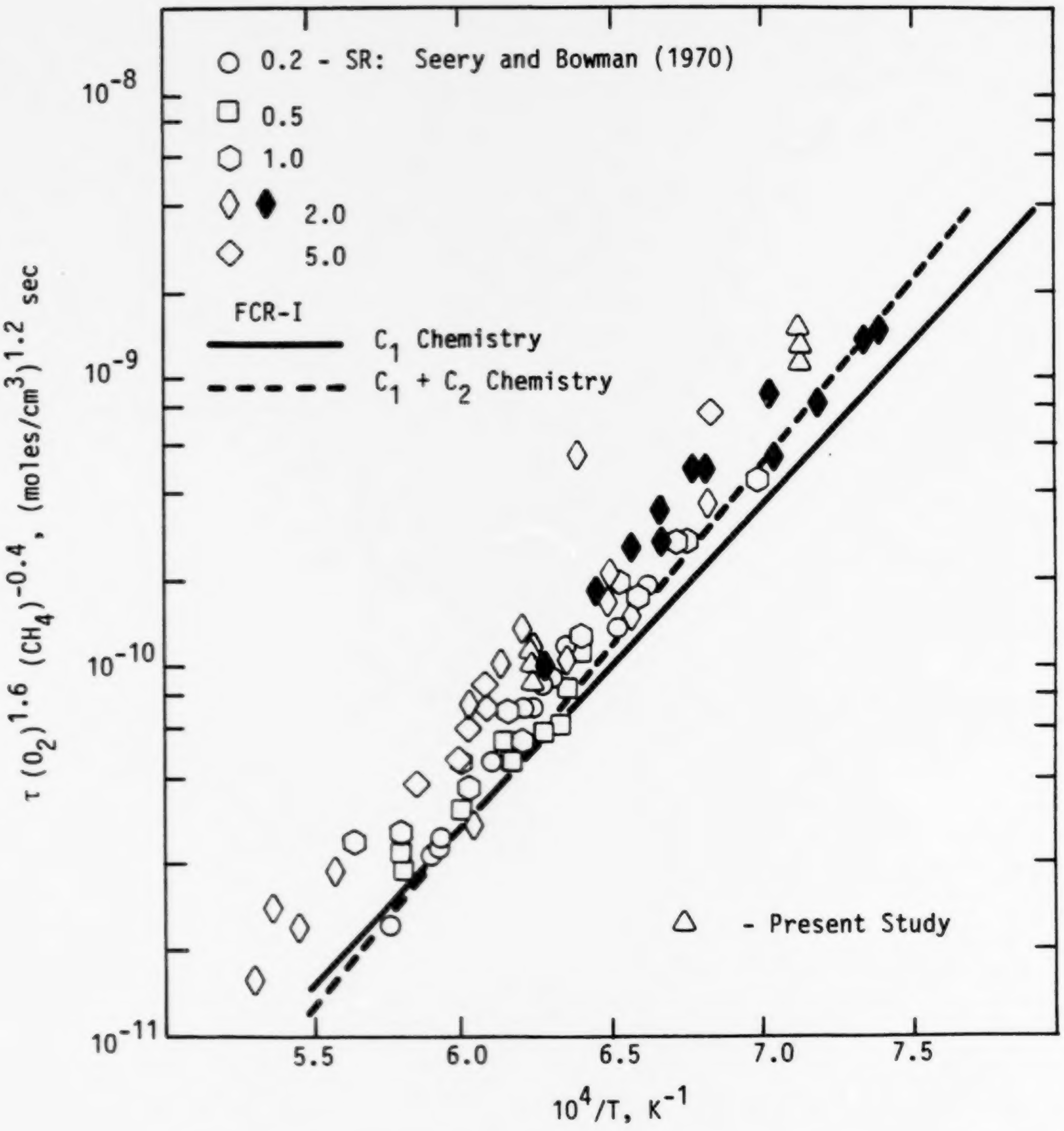

Figure 4-3. Methane-argon-oxygen ignition correlation: $Ar/O_2 = 4$.

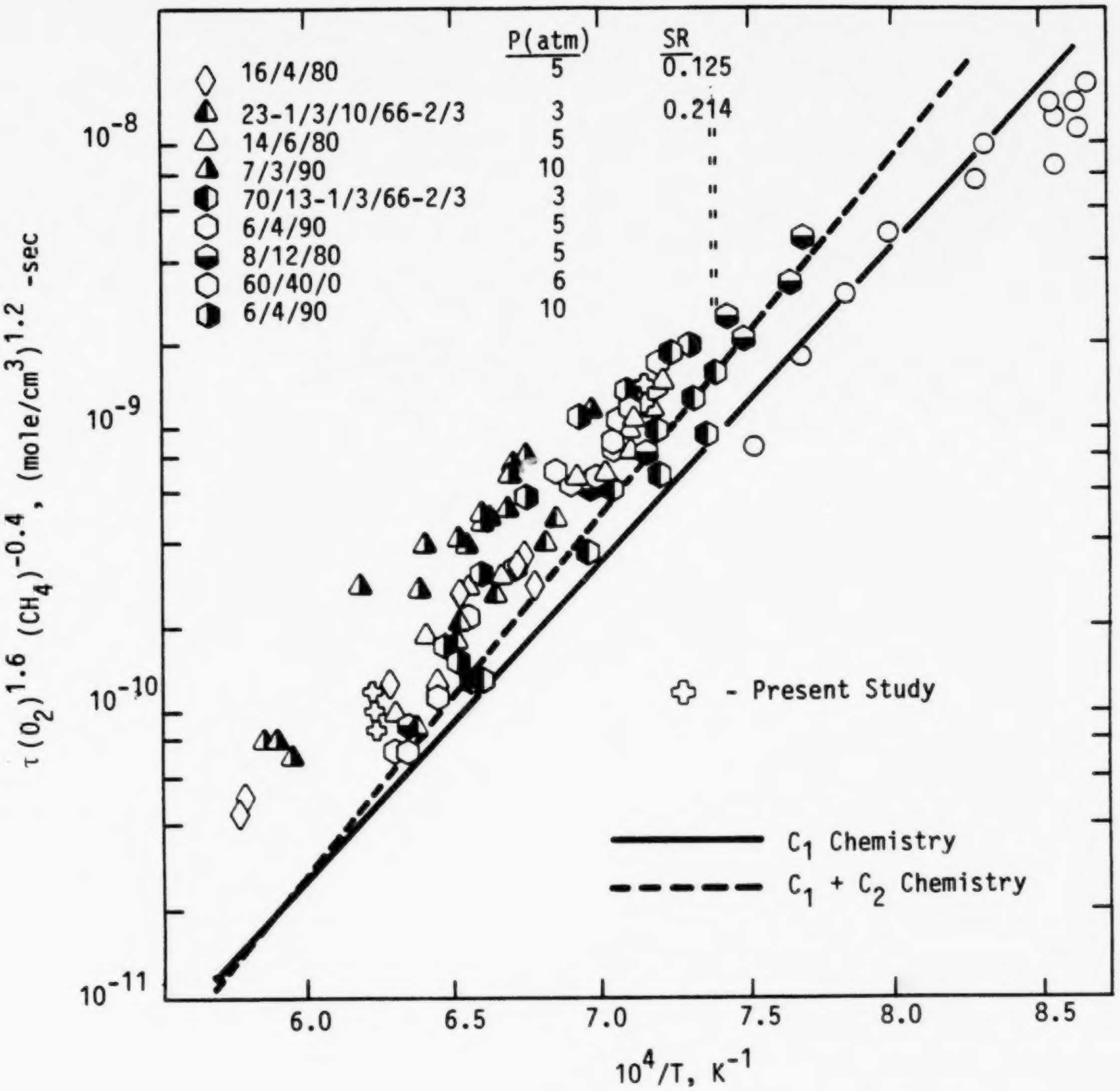

Figure 4-4. Correlation of $CH_4$-$O_2$-Ar induction times: data of Skinner and Ruehrwein (1959).

## TABLE II. PREDICTED SHOCK TUBE INDUCTION TIMES

| | Induction Time, Seconds | | | |
|---|---|---|---|---|
| Stoichiometric Ratio | 0.5 | 0.75 | 1.0 | 1.25 |
| Temp,K | | | | |
| 1400 | .0475 | .038 | .030 | .028 |
| 1600 | .0043 | .0034 | .0027 | .00255 |
| $CH_4$: $O_2$: Ar | .05/.05/.9 | .04/.06/.9 | .033/.067/.9 | .0286/.0714/.9 |

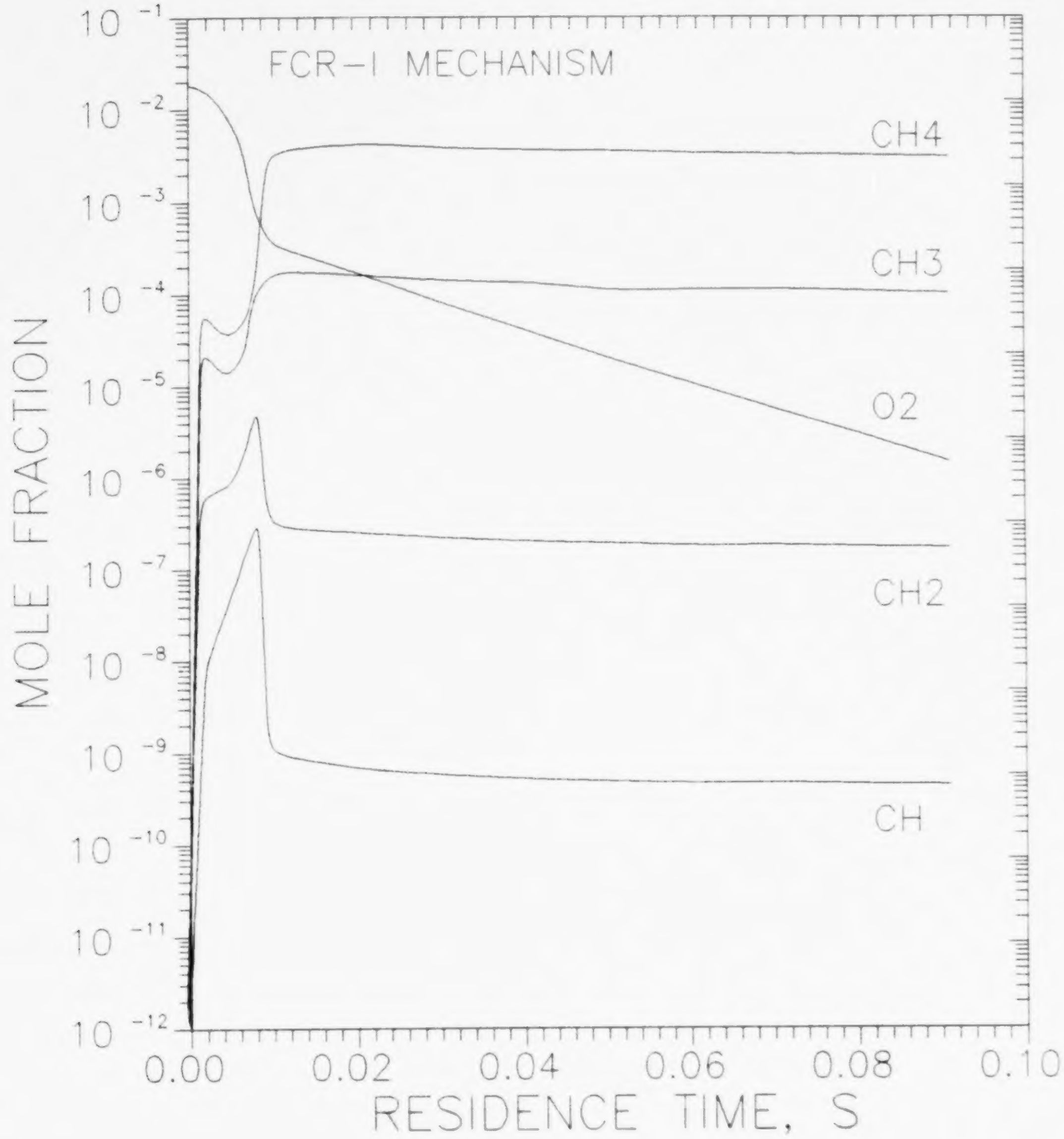

Figure 4-5. $CH_i$ and $O_2$ species profiles predicted using the FCR-I mechanism. $SR_1 = 1.1$, $SR_2 = 0.9$, $T_o = 1715$ K.

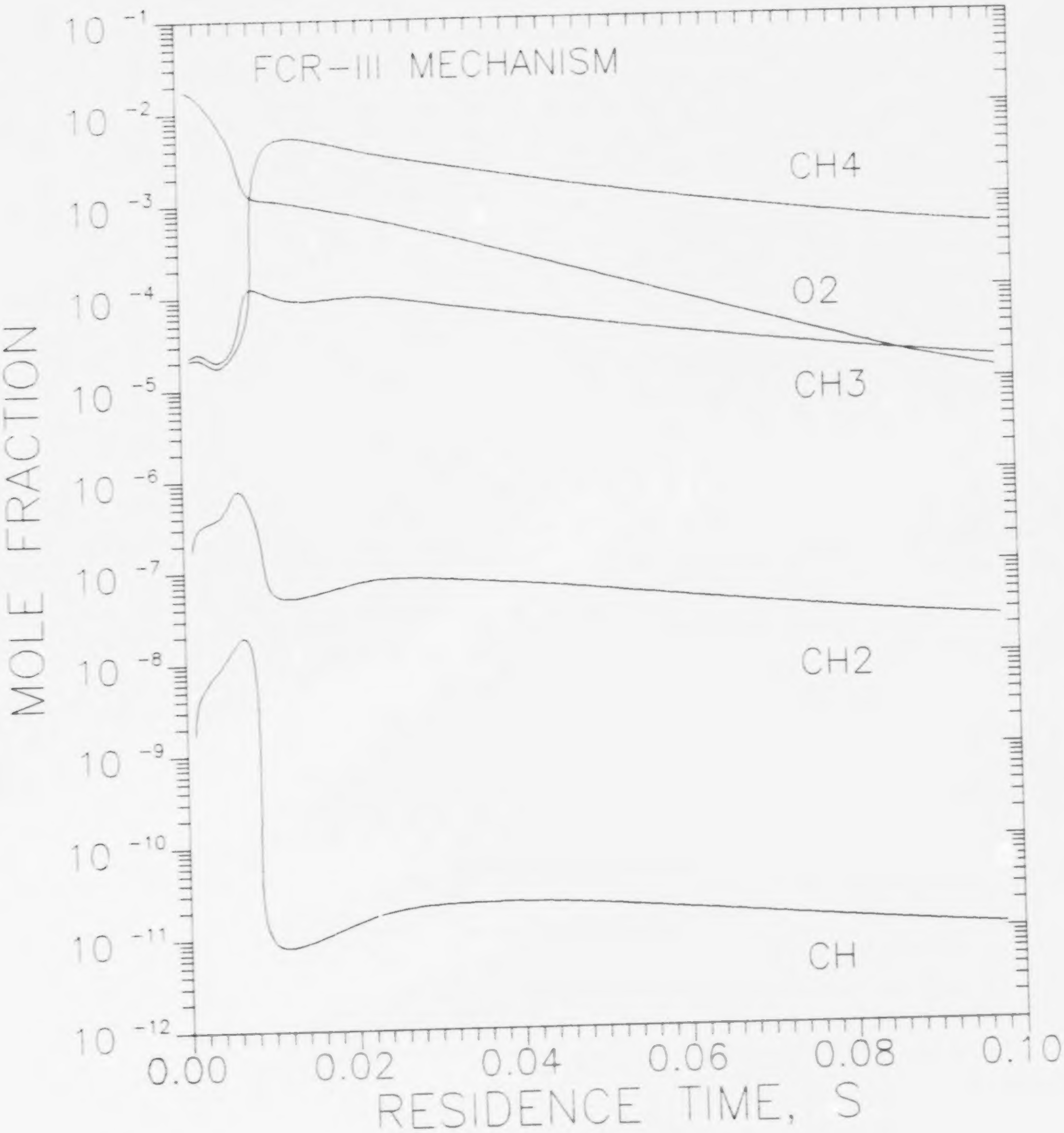

Figure 4-6. $CH_i$ and $O_2$ species profiles predicted using the present mechanism. $SR_1 = 1.1$, $SR_2 = 0.9$, $T_o = 1715$ K.

Once staging has ended, the $CH_4$ and $CH_3$ profiles level off. In both mechanisms these species are coupled because effectively 100% of the $CH_4$ destruction passes through $CH_3$. The $CH_2$ and CH profiles, on the other hand, begin to decay before the end of the staging zone. This results from the depletion of flame radicals as the $O_2$ concentration decays.

It is in the post-staging region where the two mechanisms differ most significantly. In both mechanisms, the $CH_i$ species are coupled by a set of reactions represented by

$CH_i + X = CH_{i-1} + XH$
where: $i = 1,2,3,4$
$X = H, O, OH, CH_3$

The important differences between the two mechanisms occur in the ways in which formation and destruction of the methylidyne (CH) radical occurs. In the FCR-I mechanism CH production during reburning occurs principally through

$$CH_2 + H = CH + H_2$$

$$kr = 1.2E13$$

$$CH_3 + CH_2 = CH + CH_4$$

$$kr = 2.5E11*T^{0.7}exp(-6000/RT)$$

whereas in the present mechanism

$CH_2 + H = CH + H_2$ R40
and $CH_2 + OH = CH + H_2O$ R71

predominate.

In the FCR-I mechanism, the rate of CH formation from $CH_2$ is faster than in the present mechanism for two reasons:

1. the rate constant for the $CH_2$ + H reaction is about ten times as fast in the FCR-I mechanism
2. the overall rate of the $CH_3$ + $CH_2$ reaction in the FCR-I mechanism is about 2-10 times as fast as reaction 71

The net rate of CH removal is about the same in both mechanisms. In light of the hundred-fold higher concentration predicted by the FCR-I mechanism, this implies the absence of at least one key CH-removal step. In the present mechanism, CH is removed predominantly by

$CH_4 + CH = C_2H_4 + H$ R29
$CH + CO_2 = CHO + CO$ R76
$CH + NO = CHN + O.$ R186

Reaction 76 dominates overall CH removal, accounting for 50 - 90% of net CH reaction. In the FCR-I mechanism the rates for reactions 29 and 76 are about two percent of the rates in the present mechanism. Meanwhile the combined rates of reactions 186 and 187 are the same in both reactions.

To summarize:

- Both mechanisms have the $CH_i$-species concentrations coupled through reversible H-atom abstraction reactions
- The rates of the $CH_2$ = CH reactions are about 10 times as fast in the FCR-I mechanism
- Rate constants for key CH-removal reactions are 100 times as fast in the present mechanism

## 4.3 Reburning

The previous section compared the present mechanism with the older FCR-I mechanism by using both to model methane reburning in the Hutsonville boiler. The impact of reburning on $NO_x$ (prior to burnout) is considered in this section. Figure 4-7 illustrates the $NO_x$ reduction profiles predicted by the two mechanisms for the example in the previous section. The FCR-I mechanism

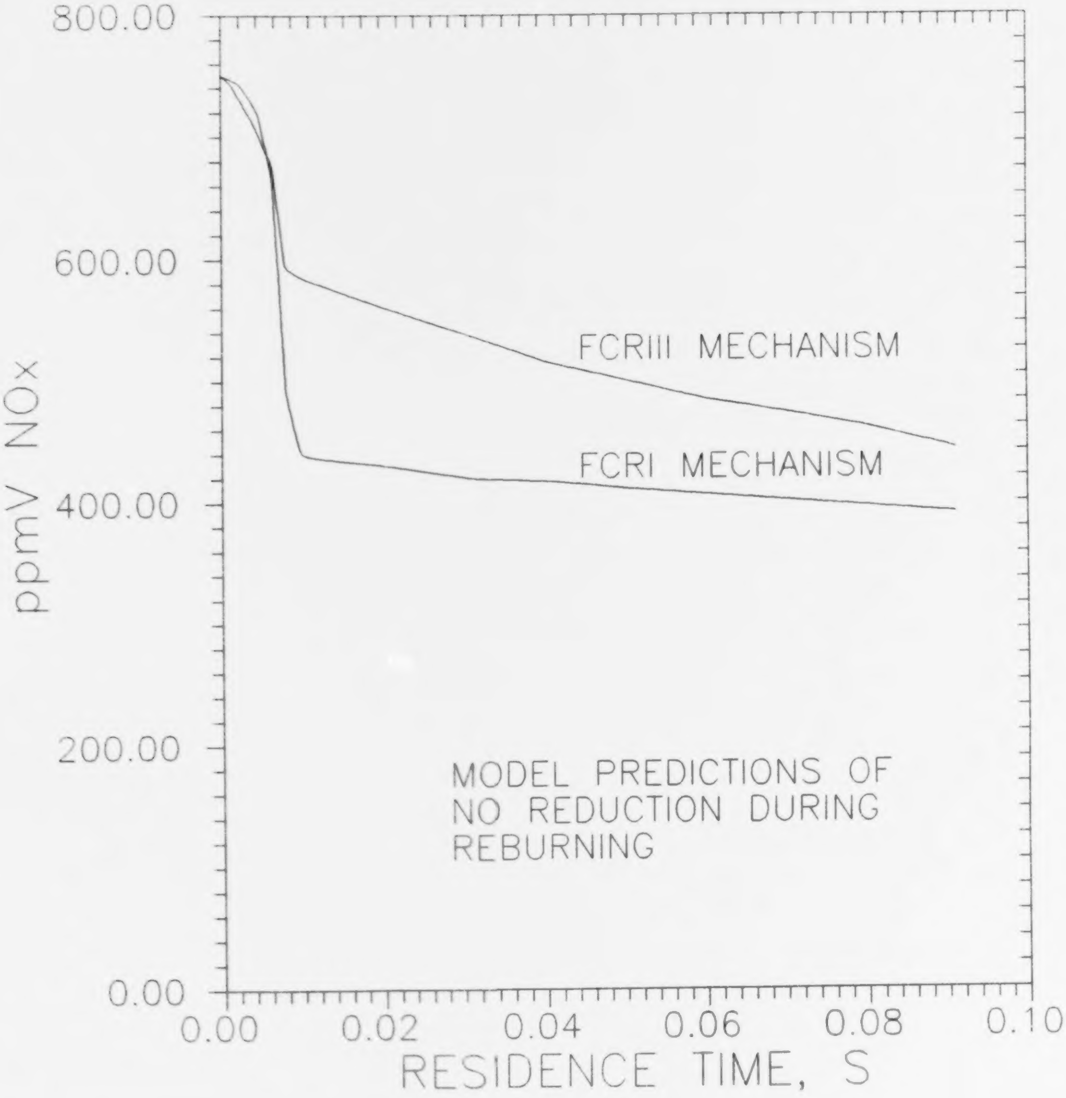

Figure 4-7. $NO_x$ concentration profiles during reburning. Predictions made using the present mechanism and the FCR-I mechanism. $SR_1 = 1.1$, $SR_2 = 0.9$, $T_o = 1715$ K.

predicts 45% $NO_x$ reduction in 50 ms, while the present mechanism shows only 30% reduction. At longer times (~1 s) the present mechanism predicts over 70% reduction of $NO_x$ while the FCR-I mechanism predicts 65% NO reduction. Experimental studies of reburning show typically 50-70% $NO_x$ reduction.

Since the present mechanism provides a somewhat better representation of combustion, why doesn't it show effective NOx reduction at short times? Figure 4-8 shows a schematic representation for NO destruction in each mechanism. The major difference between the present mechanism and the FCR-I mechanism, is shown by Figure 4-8 to lie in the reactions

$CH_2 + NO = CHN + OH$ R185
$CH + NO = CHO + N$ R186
$CH + NO = CHN + O$ R187

It was shown that the present mechanism predicts substantially lower concentrations for the CHi species, especially CH. This fact alone precludes reactions 185-187 from significantly impacting the NO concentration. However, an additional factor also arises due to reaction 112

$N + NO = N2 + O$ R112

In the FCR-I mechanism reaction 112 accounts for up to 45% of the total NO destruction. The primary source of N-atom for this reaction, however, is reaction 186. In the FCR-I mechanism the total rate for the reaction

CH + NO --- products R186,187

is the same as in the present mechanism. The difference lies in the branching ratio which is k187:k186 = 10:1 in the FCR-I mechanism. This is the inverse of the branching ratio used in the present mechanism which was discussed in Section 3.3.

At times longer than 0.1 s, the present mechanism predicts a slow, but steady decline in $NO_x$ concentration. This is accompanied by a shift in

$NO_x$-reduction chemistry from the $CH_i$ routes to the $NH_i$ routes. Much of the fixed nitrogen which is rapidly reduced by hydrocarbon fragments during fuel addition winds up as HCN and $NH_3$. As Figure 4-8 indicates, at longer times, the HCN is converted to $NH_3$ by a series of free radical interactions. The $NH_3$ serves as a reservoir for $NH_2$ production. In fact, a partial equilibrium is maintained between the $NH_i$ species. The $NH_i$ species then reduce NO to $N_2$ either directly, or through intermediate species $HN_2$ and $N_2O$.

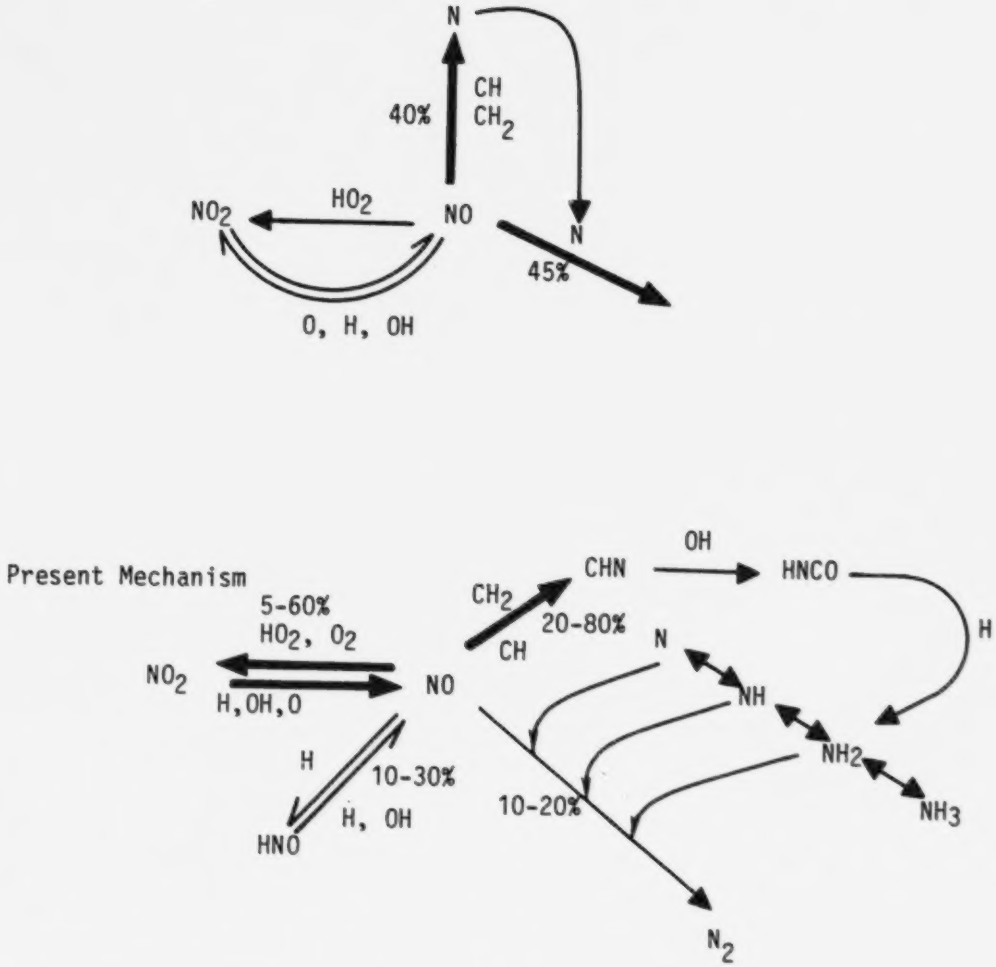
N
40%
CH
CH$_2$
NO$_2$
HO$_2$
NO
N
45%
O, H, OH
Present Mechanism
OH
CHN
HNCO
5-60%
HO$_2$, O$_2$
CH$_2$
20-80%
H
CH
N
NO$_2$
NO
H,OH,O
NH
NH$_2$
H
10-30%
10-20%
NH$_3$
H, OH
HNO
N$_2$

Figure 4-8. Schematic representation of the NO destruction routes in the FCR-I and present kinetic mechanisms. Heavy lines represent major pathways. Percentage numbers indicate total rate of NO consumption by the indicated pathway.

## 5.0 MODELING BENCH-SCALE DATA

Modeling the reburning process requires attention to the details of the physical, as well as chemical processes occuring in combustion systems. The model was applied against bench-scale data obtained in the EER Controlled Temperature Tower (CTT) in order to address some of the needs. Systematic variations of reburning parameters were applied to modeling the reburning process in order, not only to improve the model predictions, but also to provide insight into the processes occurring during reburning in practical combustion systems. Significant parameters which were investigated were:

Reburning fuel addition rate

Burnout air addition rate

Temperature change during
reburning fuel addition

Temperature change during
burnout air addition

By examining the influence of physical parameters, such as temperature profile and staging rate, the chemistry of the reburning system was found to be very sensitive. However, the uncertainty in the physical situation was not sufficient to allow the model predictions to match the data. It was necessary to assume two phenomenological chemical reactions.

### 5.1 Modeling Format

Figure 4-6 showed the behavior of the hydrocarbon species profiles during reburning fuel addition. The fuel addition time was 10 ms. As fuel entered the system the concentrations of the $CH_i$ species initially increased monotonically. After about 2 ms, however, the $CH_4$ concentration dipped momentarily, and the other methane fragment concentrations showed corresponding inflections. An analysis of the model output in that region showed that the fuel addition is quenching the radical pool by consuming H, OH, and O. As the reactions proceeded, however, the radical pool recovered with exponential growth. As a result the radical-hydrocarbon reactions soon outran the fuel addition rate. The condition quickly stabilized, however, and the $CH_4$ concentration resumed its climb

This illustrates the potential importance of the rates of fuel and air addition rates on the model predictions. Based upon this the decision was made to add both reburning fuel and burnout air at constant rates. These rates were normalized so that the time for fuel addition was 10 ms to go from SR=1.1 to SR=1.0 and the time for air addition was 10 ms to go from SR=1.0 to SR=1.25. The choice of 10 ms was arbitrary but was long enough so that the impact of staging time was small at SR=1.0.

Another significant observation was that the kinetic behavior was very sensitive to temperature. Therefore, defining the local temperature during fuel and air staging was critical. As an example, as fuel is added to a fuel-lean combustion system, the fuel is consumed initially by oxidation by the free $O_2$ present. Therefore, the temperature rises accordingly (since the time for fuel addition is fast, the burning is probable close to adiabatic.) As the local stoichiometry passes about SR = 0.96 however, endothermic pyrolysis reactions become important and further addition of fuel results in a temperature drop. Figure 5-1 shows the temperature vs stoichiometry relationship for $C_3H_8$/air flames relative to SR=1.1 (SR1). Figure 5-2 shows a schematic example of a temperature excursion during reburning fuel addition.

This presents a very complicated picture during mixing of the fuel. The approach taken to test this effect was to examine the process on a local scale and represent the fuel staging by a perfectly mixed bulk phase with a stoichiometry (hence, temperature) which changes with time. Having identified $\Delta T=f(SR-1.1)$(from Figure 5-1) and $SR=g(t)$, $\Delta T=f(g(t)-1.1)$ was then known. This $\Delta T$ was then imposed upon the temperature profile being modeled as was shown, for example, in Figure 5-2.

The impacts of both fuel-staging rate and the temperature excursion are shown in Figure 5-3. In Figure 5-3A relative $NO_x$ levels are shown at the end

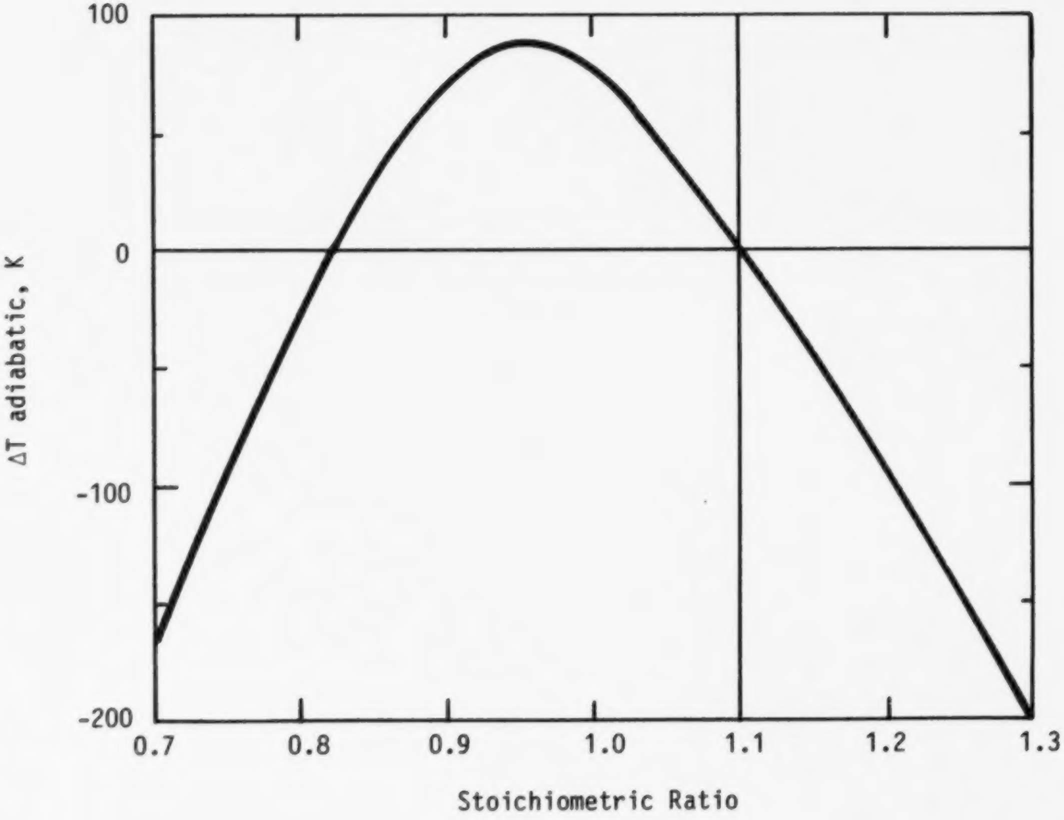

Figure 5-1. ΔT adiabatic relative to $SR_1$ = 1.1 for $C_3H_8$ in air.

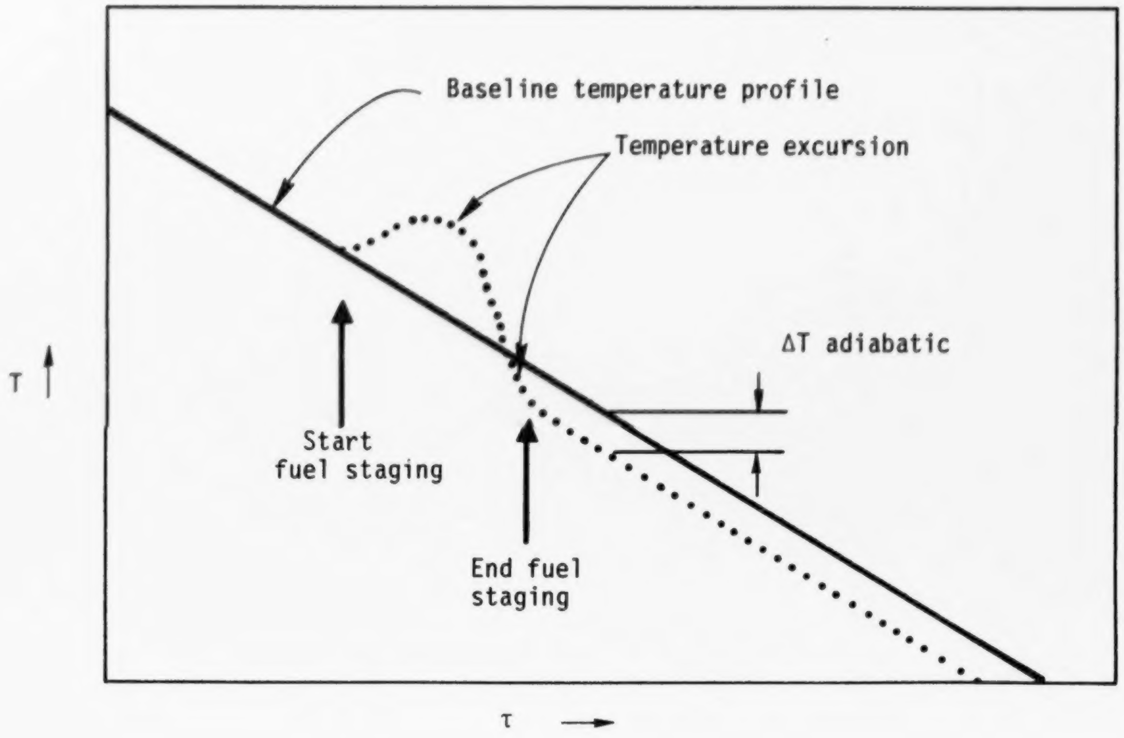
Baseline temperature profile
Temperature excursion
ΔT adiabatic
Start fuel staging
End fuel staging
T
τ

Figure 5-2. Schematic representation of the impact of staging fuel heat release on an idealized temperature profile during reburning.

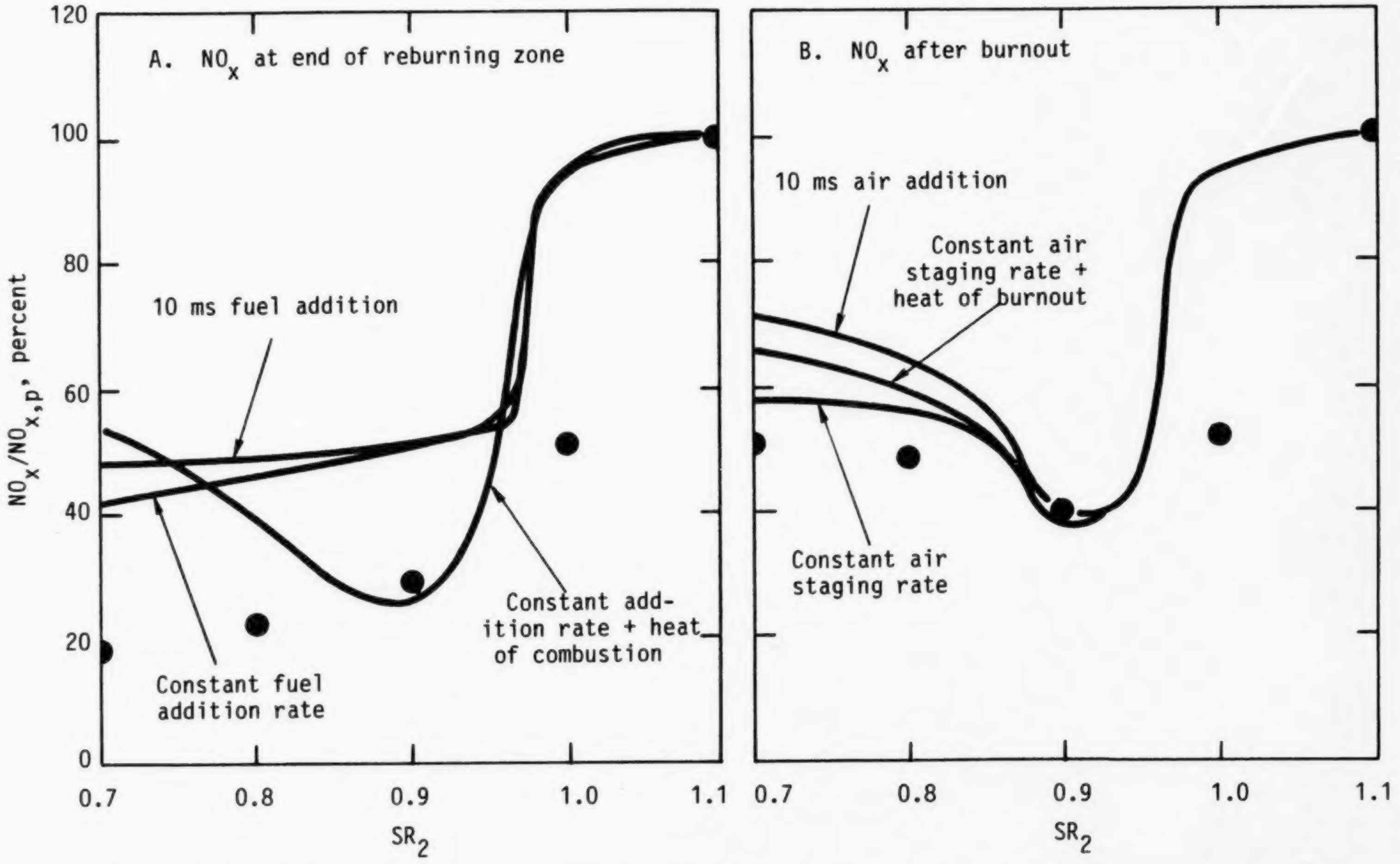

Figure 5-3. Effect of modeling format on ratio of $NO_x$ to initial $NO_x$ level: A. at the end of the reburning (fuel-rich) zone, B. After burnout, all values are corrected for the effect of dilution. $SR_1 = 1.1$, $SR_2 = 1.25$. Solid symbols represent CTT data for $C_3H_8$ reburning (Green, 1985).

of the reburning zone for $C_3H_8$ reburning. The solid symbols represent data obtained in the CTT. For fuel addition the imposition of a constant addition rate has a small but positive impact on the fit to the data. This might conceptually be viewed as a diffusion flame. As the total amount of added fuel increases the rate of burning does not change, but, rather, the burning time increases. While this is not strictly accurate, it aids in simulating the physical process of mixing within a one-dimensional model.

Adding the temperature excursion to the fuel-addition case improved the overall fit to the data. At SR=0.7 the relative $NO_x$ level is higher than that predicted in the fuel-leaner cases. This is attributed to the rather large temperature drop and resultant depression of the radical concentrations and rates of all reactions.

After burnout the effect of a constant air staging rate is more dramatic. In this case the fit to the data is both quantitatively and qualitatively improved. When the temperature excursion of burnout is also considered the result is somewhat of a compromise, although still better than the base case.

## 5.2 Phenomenological Modeling

Even accounting for the environmental effects as in the previous section, the model did not adequately predict the concentrations of the reduced nitrogen species, $NH_3$ and HCN. Figure 5-4 compares the predicted concentrations of these species with measurements taken in the CTT. At SR=0.7 the discrepancy between the measured and predicted HCN concentrations is larger than the $NO_x$ deficit shown in Figure 5-3A. Therefore, further reduction of $NO_x$ is not sufficient to provide the measured HCN concentration. In order to produce this much HCN there must also be a mechanism for fixation of $N_2$.

A review of the literature found only two mechanisms for direct fixation of molecular nitrogen to reduced nitrogen species in combustion systems. These are:

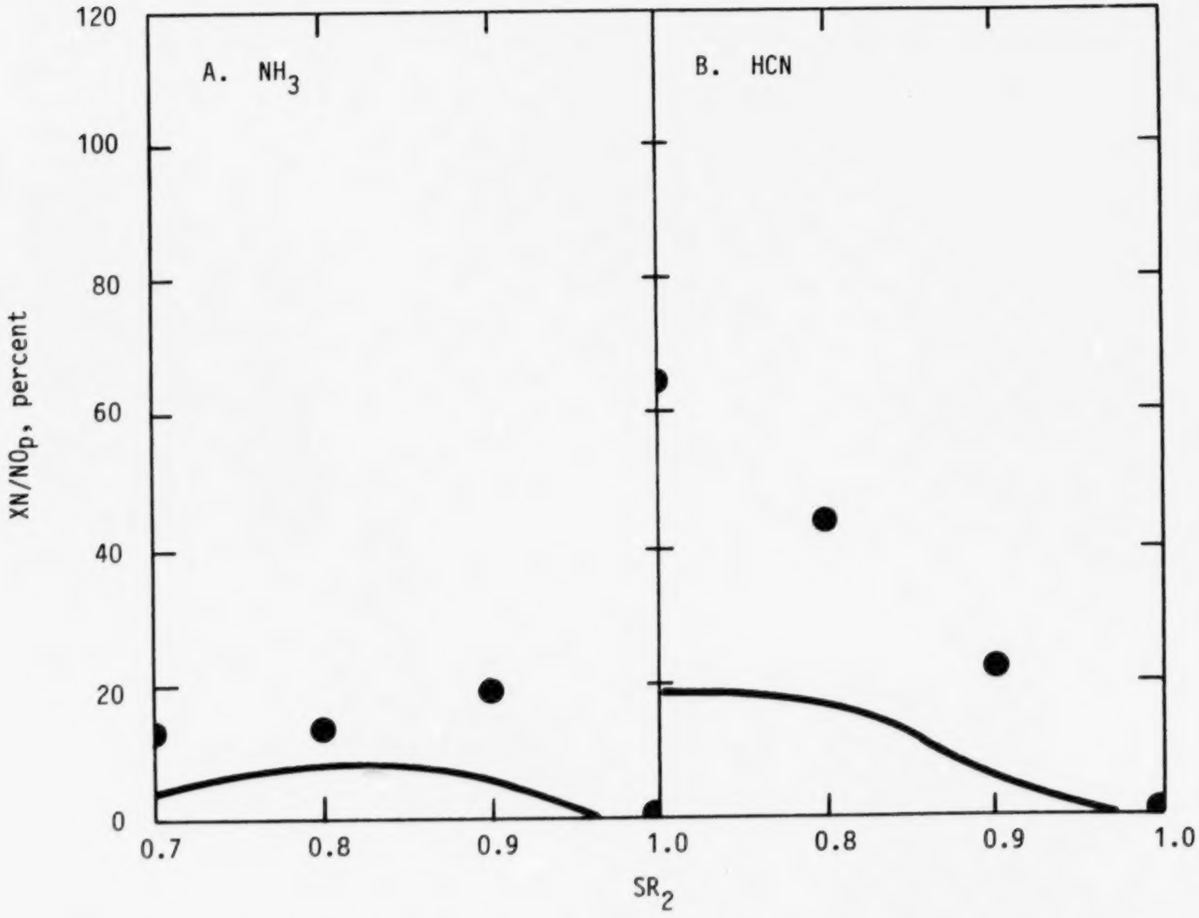

Figure 5-4. Model predictions of relative concentrations of A. $NH_3$ and B. HCN at the end of the reburning (fuel rich) zone. Solid symbols are the data of Greene (1985) $SR_1 = 1.1$.

$CH + N_2 = HCN + N$ R174

and $CH_2 + N_2 = HCN + NH$ R171

The rates of both of these reactions are fairly well known and they both are accounted for in the present mechanism.

What the mechanism lacks is a reaction or set of reactions which will accomplish two things:

. Reduce NO at SR=0.7 but not at SR=0.9
2. Fix $N_2$ more rapidly at SR=0.7 than at SR=0.9

Both of these criteria require that the reaction(s) be faster at lower stoichiometric ratios, and, hence, lower temperatures. This means that either the reaction(s) must have a negative activation energy, or must involve species which exist under fuel-rich stoichiometries but not near stoichiometric or fuel-lean conditions ($CH_2$ and CH radicals do not meet this criterion.)

Acetylene and the ethynyl radical both meet the latter requirement. While both of these species are integral to the oxidation pathways of most hydrocarbons, neither accumulates in appreciable concentrations at stoichiometries leaner than about SR=0.9. Two reactions which are proposed and their a priori rate expressions are:

$C_2H_2 + NO = CHO + HCN$ $k = 8.133E5*\exp(+14140/RT)$

$H_{rxn} = -33.1$ kcal/mol

$C_2H + N_2 = CN + HCN$ $k = 1.26E12*\exp(-21000/RT)$

$H_{rxn} = +2.3$ kcal/mol

The enthalpies of reaction were obtained from Kee (1987).

The rate for the attack of acetylene on NO was estimated merely on the basis of what was needed in order to produce the experimentally observed NO reductions at different SR2s. The rate for ethynyl attack of $N_2$ was estimated by applying the methods described by Benson (1976). This involved first evaluating the energy and entropy levels of the reaction pathway through the adduct and the estimated transition states. The entropy levels provided estimates for the Arrhenius parameter and the energy levels were used to calculate the activation energy .

These reactions were appended to the reaction mechanism shown in Table I and evaluated against the CTT reburning data. Their rate expressions were then adjusted parametrically in order to best fit the data over the range of SR2=1.0 to SR2=0.7. The resulting "best fit" rate expressions are:

$$C_2H_2 + NO = CHO + HCN \qquad k = 2.2E5*\exp(+14140/RT)$$

$$C_2H + N_2 = CN + HCN \qquad k = 1.26E12*\exp(-25000/RT)$$

Figure 5-5 shows the secondary (reburning) zone concentrations of $NO_x$, $NH_3$, and HCN predicted with the two phenomenological reactions included in the reaction mechanism. The prediction of HCN behavior is very good over the range of stoichiometries shown. The trend of $NH_3$ concentration is quite good although the predicted values are generally low. Predictions of NOx concentrations are excellent except at SR=1.0. This discrepancy may be due to both experimental error and the sensitivity of the model predictions at stoichiometries near 1.0.

Another reaction which has not yet been considered is:

$$C_2H + NO = \text{Products}$$

There are two likely adducts resulting from linear addition of ethynyl to NO, depending upon whether the radical carbon atom attacks the nitrogen or the oxygen atom in NO. In addition, attack of the N-O bond by the radical carbon atom and attack of the C-C bond by either atom of NO are possible reaction routes. Among the possible product distributions are:

- HCN + CO
- CHO + CN
- CH + NCO

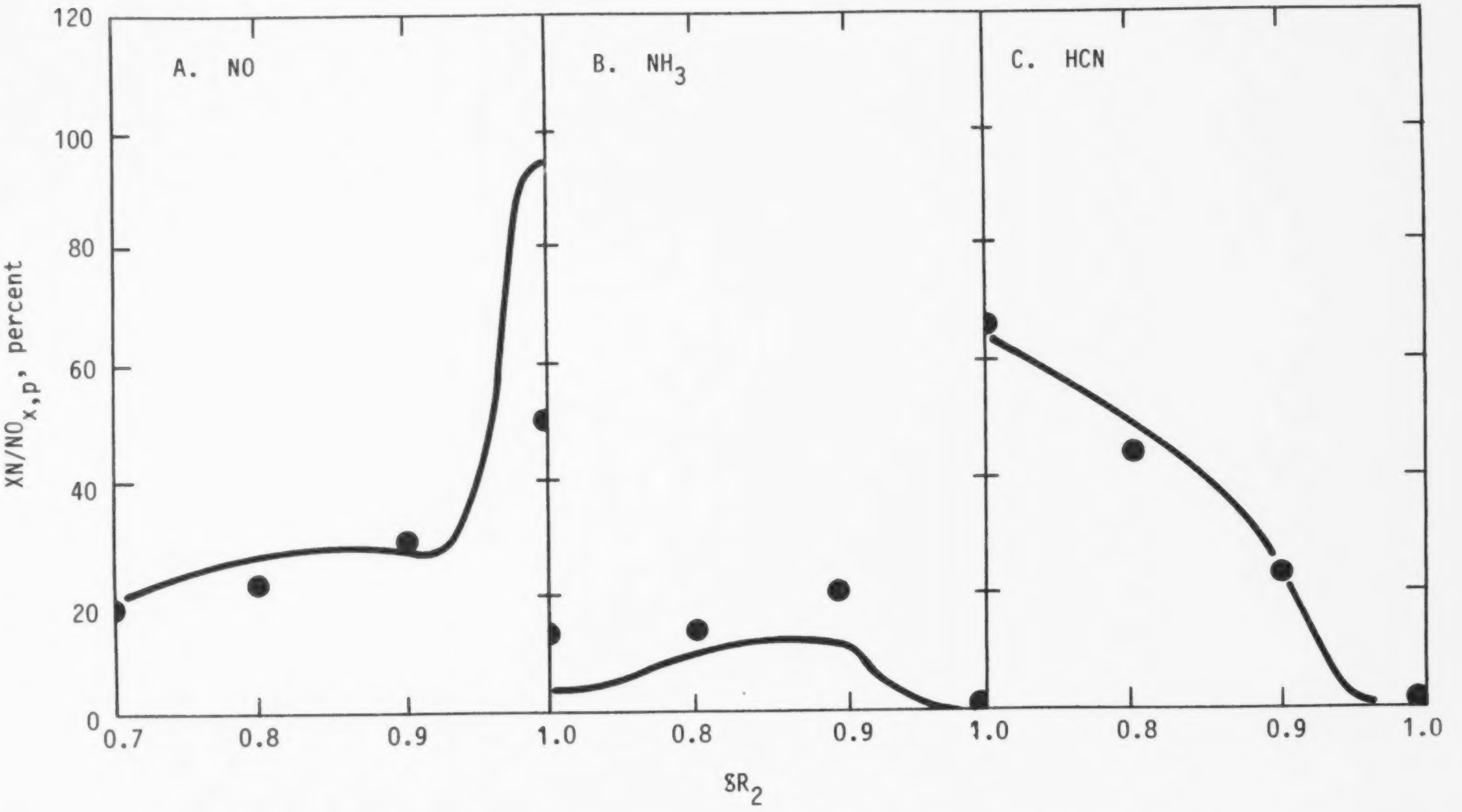

Figure 5-5. Model predictions of relative concentrations of A. NO, B. NH$_3$, C., HCN at the end of the reburning (fuel-rich) zone. Solid symbols are CTT data (Greene, 1985). SR$_1$ = 1.1. Phenomenological reactions included in mechanism.

## 5.3 Fuel Addition Rate

The impact of varying the fuel addition rate on model predictions was again studied using the appended mechanism. Results of this variation on $NO_x$ and TFN are shown in Figure 5-6. Changing the fuel addition rate within the model does not correspond to a change in mixing rate per se. There is no strict analogy between the addition rate in a one-dimensional model and mixing in a three dimensional combustion system. It has more to do with the rate at which the fuel heats up and becomes available to react with the bulk phase species. The reason for investigating addition rate is to test the modeling format.

The effect of fuel addition rate on the model predictions is straightforward. At shorter addition times the $NO_x$ and TFN concentrations are slightly higher. At longer times, the concentrations are not only lower, but the fit is slightly improved at stoichiometries approaching SR2=1.0.

One possible impact of a slower fuel addition rate is related to mixing. Namely, a lower mixing rate implies that some of the fuel enters the system at a lower temperature. In general, lower temperature means slower reaction rates and lower radical concentrations. However, a restricted rate of fuel addition, as in Figure 5-6, also prevents runaway growth of the radical pool and resultant oxidation of N-species to NO. This accounts for the improved $NO_x$ reduction at longer addition times within the range represented in the figure.

The simulation of mixing in one-dimensional modeling is a formidable problem. One approach which may be effective is to treat a combustion system as a two-dimensional array of stream tubes. Each stream tube can then be modeled as a one-dimensional time-variant reactor. This approach allows a finite number of cases to be evaluated by the one-dimensional model. The results of these cases then can be combined analytically through the appropriate choice of two-dimensional matrices to simulate an infinite number of time-invariant three-dimensional reacting systems.

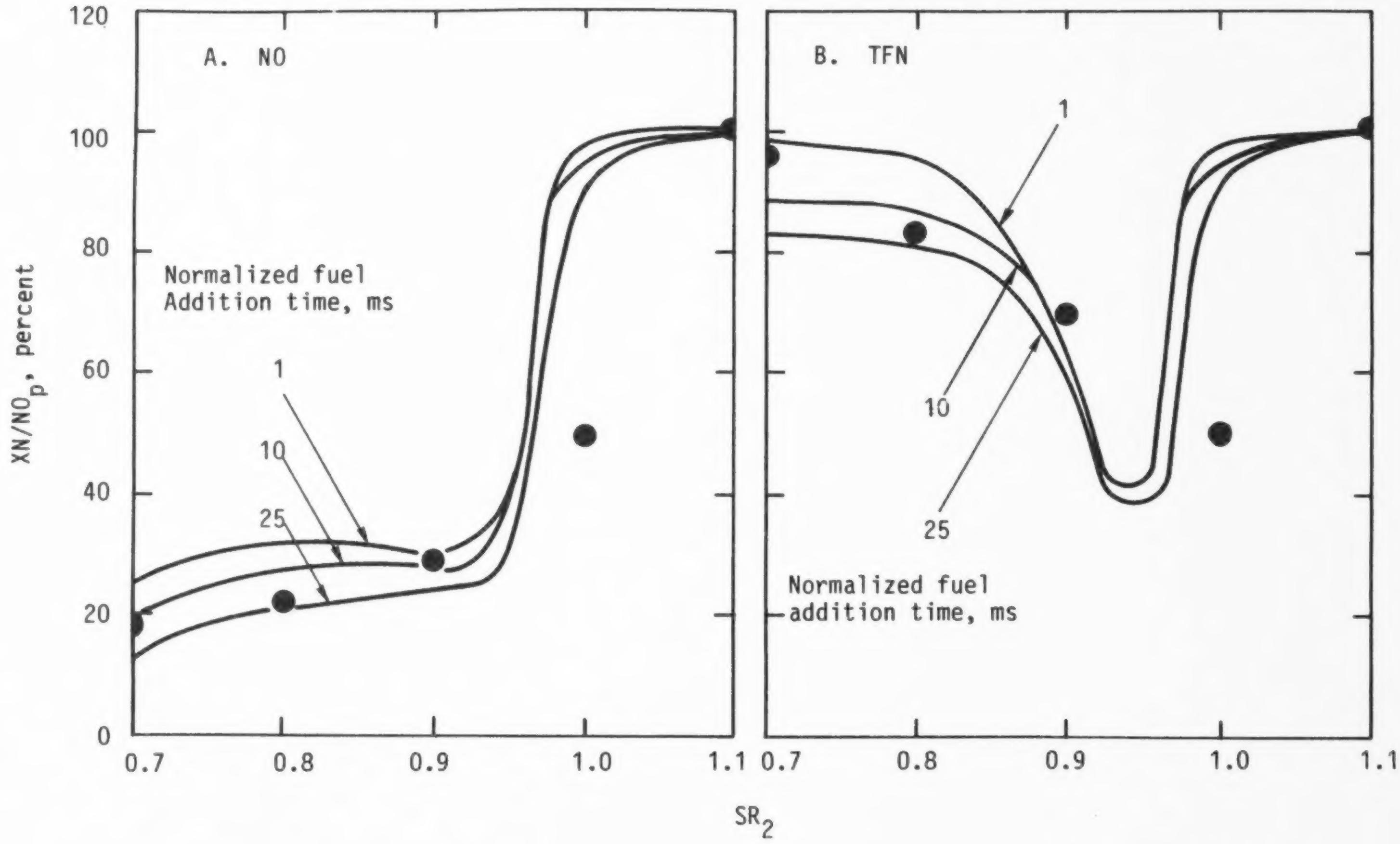

Figure 5-6. Impact of normalized fuel staging time on A. NO, B. TFN at the end of the reburning (fuel-rich) zone. $SR_1 = 1.1$. $C_3H_8$ reburning. Solid symbols represent CTT data (Greene, 1985).

## 5.4 Burnout $NO_x$ Predictions

The chemistry occurring during burnout air addition is complicated. A large volume of air relative to the total system volume is needed to effect burnout. This results in a quench of the radical species concentrations followed by reignition and a series of reactions which occur at progressively leaner stoichiometries. Initially the radical species concentrations rise and reignite the reburning reactions responsible for $NO_x$ reduction. However, the excess oxygen and increasing radical levels soon begin to oxidize the remaining fixed nitrogen species.

The model prediction for $NO_x$ concentration after burnout are shown in Figure 5-7. This model prediction curve shows the qualitative features of the data. However, the predicted concentrations of $NO_x$ vs SR2 are too high. This indicates that the predicted oxidation of the remaining fixed nitrogen species is too efficient. An analysis of the reactions taking place indicates that about 80% of the HCN at the end of the reburning zone is oxidized to NO.

The important chemical pathways for HCN and $NH_3$ destruction during burnout are shown in Figure 5-8. All of the HCN and $NH_3$ pass through the $NH_i$ radical pool. The $NH_i$ species may then be oxidized to $N_2$ by reaction with NO or may be oxidized directly to NO themselves. The ratio of NO reduction to NO production through these reactions is sensitive, not only to the specific reaction rates, but also to the modeling conditions and to the modeling format. Further adjustment to the rates of the reactions represented in Figure 5-8 may resolve the major discrepancies in the model predictions shown in Figure 5-7.

## 5.5 Summary

A comparison of the model and kinetic mechanism with bench-scale data obtained in the EER Controlled Temperature Tower (CTT) was used to investigate the importance of several parameters in the modeling format and to test two proposed phenomenological chemical reactions. The results show the importance of the heat release during reburning. They also indicate that the fuel and

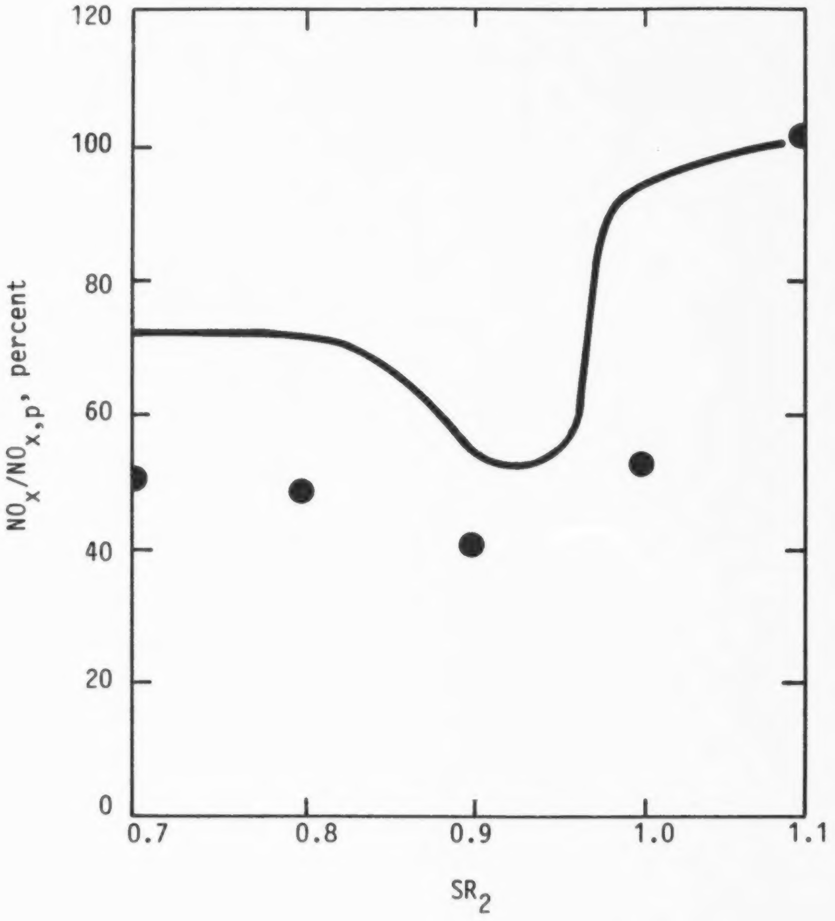

Figure 5-7. $NO_x$ after burnout. $C_3H_8$ reburning. Solid symbols represent the data of Greene (1985). $SR_1 = 1.1$, $SR_3 = 1.25$, 10 ms normalized fuel addition time. Phenomenological reactions included in kinetic mechanism.

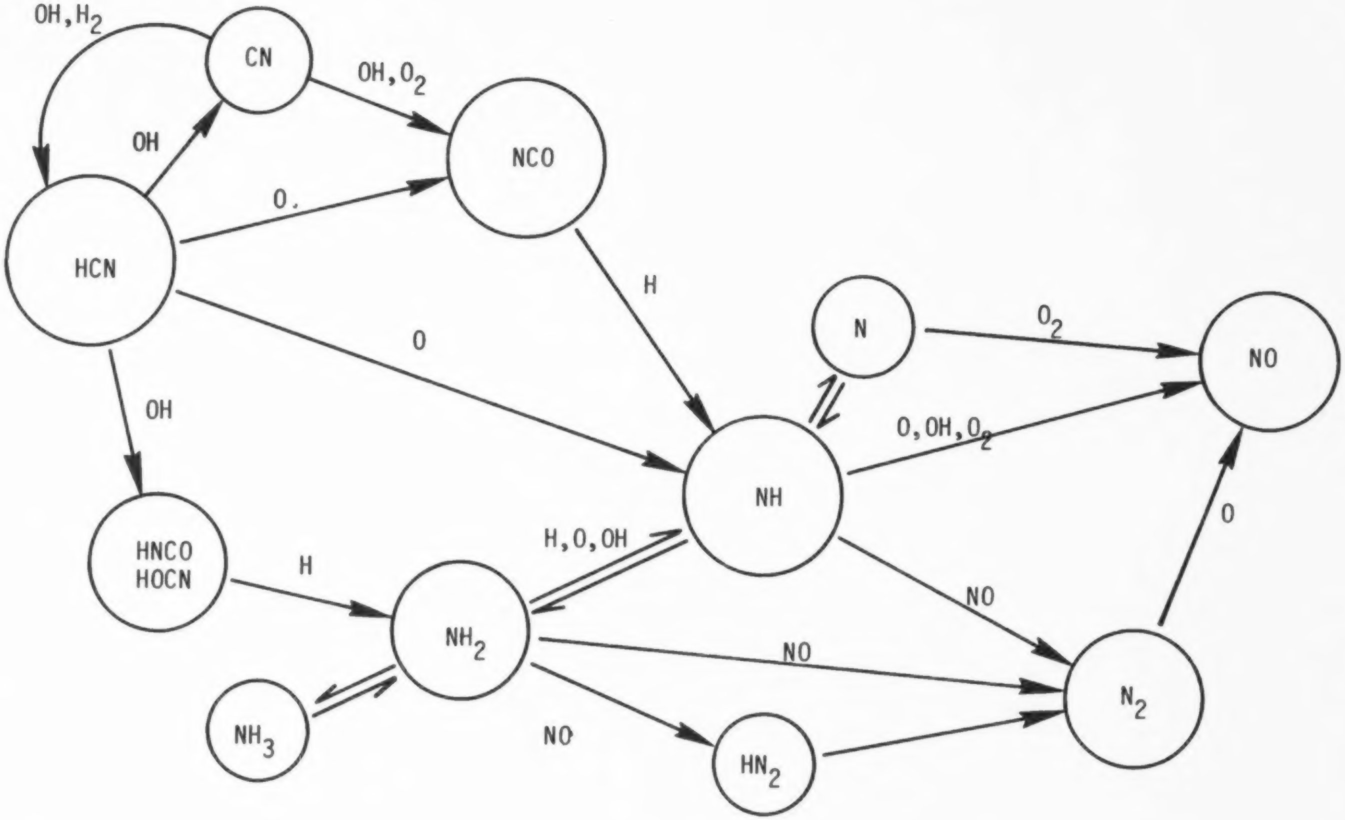
OH, $H_2$
CN
OH, $O_2$
OH
NCO
HCN
O.
H
O
N
$O_2$
NO
OH
O, OH, $O_2$
NH
HNCO
HOCN
H
H, O, OH
$NH_2$
NO
O
NO
$N_2$
$NH_3$
NO
$HN_2$

Figure 5-8. Reduced nitrogen species oxidation pathways during air staging from the reburning zone.

air addition rates are important parameters. This implies that mixing is a critical experimental variable and may have significant impact on the way in which scale-up of the reburning process is carried out.

The impact of mixing upon a three-dimensional system was not evaluated. However, an approach was outlined by which one-dimensional modeling may be used to predict reburning in non-well-mixed systems.

Two phenomenological reactions were used to fit the TFN predictions in the reburning zone to the CTT data. The fit was good for the HCN and $NO_x$ predictions, but was low for the $NH_3$, although the qualitative features were correct. The model did not accurately predict the data at SR2=1.0. This may be in part due to uncertainties in the data and also due to the sensitivity of the model predictions at stoichiometries near 1.0. Further adjustment of key reaction rates may suffice to resolve the discrepancy between the model predictions and the data.

The chemistry and kinetics of reburning are impacted by temperature, stoichiometry, mixing , and staging rate, to name a few. This makes reburning a very challenging modeling task.

## 6.0 CONCLUSIONS AND RECOMMENDATIONS

The development of a gas-phase kinetic mechanism is necessarily an open-ended task. As new kinetic data arise it is sensible and prudent to incorporate them into existing mechanisms. It is also necessary; for while a mechanism may be adequate for a time, to model a process, as new questions arise so will obsolescence.

The kinetic mechanism developed here represents the current state of knowledge in homogeneous combustion modeling. The rate data are a compilation of the most reliable and up-to-date reviews available in the field of gas-phase chemical kinetics. By accounting for environmental factors and with the addition of two phenomenological reactions the present mechanism is able to adequately model NOx destruction during the reburning process.

The mechanism is also an improvement over a previous mechanism developed under the FCR-I program. It provides a more realistic picture of hydrocarbon combustion under reburning conditions. The new mechanism predicts levels of $NO_x$ reduction during reburning of the same order as those observed experimentally. The ability of the earlier mechanism to do so was based upon several rate estimates which are now no longer considered valid and therefore misleading. The main value of the present mechanism will not be in making quantitative predictions of $NO_x$ reduction, however. Rather, it will be a valuable tool for predicting the trends of reburning behavior and generalizing the reburning process at different scales.

In summary, several things were required in order to develop the mechanism and carry out the modeling efforts described in this program:

- Reliable rate data and references
- Reliable fundamental and bench-scale data against which to compare the model and mechanism
- Computer programs to assist in the organization and selection of rate data

- Understanding of the complexities involved in the reburning process

Several points can be made based upon the experience gained during this program.

1. Real processes result from complex coupling of fundamental processes, i.e. mixing, heat transfer, diffusion, etc. These can be effectively modeled one-dimensionally if certain key parameters can be correctly identified. The key parameters will vary between different experimental or full-scale configurations.

2. Physical processes (mixing, heat transfer, etc.) set the environment for the chemistry.

3. Chemistry is the means of $NO_x$ removal, but chemistry can modify the physical environment (e.g. through heat release during combustion.)

4. Development of the kinetic mechanism was only one step toward developing a valid model of the reburning process. Understanding the physical processes and accomodating them in the modeling format was an equally important aspect in not only modeling reburning, but also in deciding where changes could be made in the mechanism itself.

# 7.0 REFERENCES

Bartok, W., V.S. Engleman, R. Goldstein and E.G. del Valle. AIChE Symp. Ser. 126,(1972) 68, 30.

Benson, S.W. "Thermochemical Kinetics" 2nd ed. (1976) John Wiley and Sons, Inc, NY.

Benson, S.W. and H.E. O'Neil "Kinetic Data On Gas-Phase Unimolecular Reactions" NSRDS-NBS 21, NTIS No. PB 191956, February, 1970

Berman, M.R., J.W. Fleming, A.B. Harvey, and M.C. Lin proceedings: Nineteenth Symposium (Intl.) on Combustion; (1982) The Combustion Institute, Pittsburgh, PA, p.73.

Blawens, J., B. Smets and J. Peeters. proceedings: Sixteenth Symposium (Intl) on Combustion; (1977) The Combustion Institute, Pittsburgh, PA, p. 1055.

Bohland, T. and F. Temps. Ber Bunsenges Physik Chem. (1984) 88, 459.

Frank, P., K.A. Bhaskaran, and Th. Just. presented at The Twentieth Symposium (Intl.) on Combustion; The University of Michigan, Ann Arbor, August 12-17, 1984.

Glarborg, P., J.A. Miller and R.J. Kee. Paper WSS/CI 1-5B. Presented at the Joint Technical Meeting, San Antonio, TX, April 22-23, 1985.

Glarborg, P., J.A. Miller and R.J. Kee. Combustion and Flame (1986) 65, 177.

Greene, S.B., S.L. Chen, W.D. Clark, M.P. Heap, D.W. Pershing and W.R. Seeker. Bench-Scale Process Evaluation of Reburning and Sorbent Injection for In-Furnace $NO_x/SO_x$ Reduction. EPA-600/7-85-012 (NTIS PB85-185890). U.S. Environmental Protection Agency. March 1985.

Grillo, A. and M.W. Slack. Combustion and Flame (1976) 27, 377.

Hanson, R.K. and S. Salimian in "Combustion Chemistry", W.C. Gardiner, Jr., Ed.; 1984, Springer-Verlag, New York Inc., p.361.

Hwang, S.M., W.C. Gardiner, Jr., M. Frenklach and Y. Hidaka. Combustion and Flame (1987) 67, (1), 67.

Kau, C.J., M. P. Heap, W. R. Seeker and T.J. Tyson. Fundamental Combustion Research Applied to Pollution Formation Volume IV. Engineering Analysis. EPA-600/7-87-027 (NTIS PB88-144001). U.S. Environmental Protection Agency, December 1987.

Kee, R.J., F.M. Rupley, and J.A. Miller. The Chemkin Thermodynamic Data Base (1987), SAND87-8215: Sandia National Laboratories.

Lyon, R.K. Preprints: American Chemical Society; Division of Fuels Chemistry (1987), 32 (4), 433.

Matsui, Y. and T. Nomaguchi. Combustion and Flame (1978) 32, 205.

Michael, J.V., J.W. Sutherland and R.B. Klemm. Int. J. Chem. Kinet. (1985) 17, 315.

Myerson, A.L., F.R. Taylor and B. G. Faunce. proceedings: Sixth Symposium (Intl.) on Combustion; (1957) The Combustion Institute, Pittsburgh, PA, p.154.

Myerson, A.L. proceedings: Fifteenth Symposium (Intl) on Combustion; (1975) The Combustion Institute, Pittsburgh, PA, p.1085.

Patry, M. and Engel, G. Compt. Rend. (1950), 231, 1302.

Peeters, J. and C. Vinckier. proceedings: Fifteenth Symposium (Intl) on Combustion. (1975) The Combustion Institute, Pittsburgh, PA, p 969.

Reed, R.D. "Process for the Disposal of Nitrogen Oxide." John Zink Company, U.S. Patent 1274637, 1969.

Seeker, W.R., M.P. Heap, T.J. Tyson, J. C. Kramlich and T. L. Corley. Fundamental Combustion Research Applied to Pollution Formation. Volume I: FCR Program Overview and Gas-Phase Chemistry. EPA-600/7-85-048 (NTIS PB86-122660). U.S. Environmental Protection Agency, October 1985.

Seery, D.J. and C.T. Bowman. Combustion and Flame (1970) 14, 34.

Skinner, G.B. and R.A. Ruehrwein. J. Phys. Chem. (1959) 63, 1736.

Takahashi, Y., N. Murakami, T. Kawamura, H. Haneda, K. Muraishi, M. Sakai, T. Sengoku, T. Kunimoto, A. Hirayama, and S. Kaneko. Presented at the U.S. - Japan $NO_x$ Information Exchange; Tokyo, Japan, May, 1981.

Tsang, W. and R.F. Hampson. J. Phys. Chem. Ref. Data (1986) 15 (3), 1087.

Tsuboi, T. and H. Gg. Wagner. proceedings: Fifteenth Symposium (Intl.) on Combustion; (1975) The Combustion Institute, Pittsburgh, PA, p.833.

Warnatz, J. in "Combustion Chemistry:, W.C. Gardiner, Jr., Ed.; (1984), Springer-Verlag, New York Inc., p.197.

Wendt, J.O.L., C.V. Sternling and M.A. Matovich. proceedings: Fourteenth Symposium (Intl.) on Combustion; (1974), The Combustion Institute, Pittsburgh, PA, p. 897.

Westbrook, C.K., and F.L. Dryer. Prog. Energy Combust. Sci. (1984) 10, 1.

Zellner, R. J. Phys. Chem. (1979) 83, 18.

# APPENDIX A

## COMPILATION OF RATE DATA AND ARRHENIUS PLOTS OF RATE CONSTANTS.

This appendix contains the compilation of rate data which were reviewed in the development of the reburning kinetic mechanism. The format of this appendix is as follows:

- The appendix is broken into 10 subsections according to the elements participating in the reactions (excluding chaperones). These are

  1. $H_2O_2$
  2. CO
  3. CH
  4. CHO
  5. NO
  6. NH
  7. HNO
  8. NCO
  9. HCN
  10. HNCO

- Each subsection consists of two parts. The first part is a compilation of rate expressions and references. A notation is provided in the table to indicate whether the rate expression is for the forward or reverse direction of the reaction as written. The second part consists of the Arrhenius plots for each reaction. Each plot represents a single reaction and contains all of the data reviewed for that reaction. The individual curves are not labeled, but may be identified using the information in the preceding table for that subsection.

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*---------------------------------------------------------------------------------*
| File: H2O2MECH.DAT                                                              |
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*---------------------------------------------------------------------------------*

 1H2    + 1O2            = 1HO    + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                   1.7E+13 0.000 47.780  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                     2.5E+12 0.000 39.000  1000.0  2000.0
Seeker, et al. 1985
Baulch, et al. 1972                     5.5E+13 0.000 47.780  1000.0  2000.0

 1H2    + 1O             = 1HO    + 1H
Forward Rate Parameters:
Seeker, et al. 1985                     1.8E+10 1.000  8.830   400.0  2000.0
Glarborg, et al. 1985
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, J. 1984                        1.5E+07 2.000  7.550   300.0  2500.0

 1H2    + 1HO            = 1H2O   + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   1.2E+09 1.300  3.630  1000.0  2000.0
Glarborg, et al. 1986
Warnatz, J. 1984                        1.0E+08 1.600  3.300   300.0  2500.0
Westbrook and Dryer                     2.1E+13 0.000  5.150   300.0  2500.0
Seeker, et al. 1985                     1.1E+09 1.300  3.650  1000.0  2000.0

 1H     + 1H     + 1M    = 1H2    + 1M     +
Reverse Rate Parameters:
Glarborg, et al. 1985                   2.2E+12 0.500 92.600  1000.0  2000.0

 1H     + 1H     + 1AR   = 1H2    + 1AR
Forward Rate Parameters:
Seeker, et al. 1985                     9.0E+17-1.000  0.000  1000.0  2000.0
Warnatz, J. 1984                        6.4E+17-1.000  0.000  2500.0  3000.0
Glarborg, et al. 1986                   1.0E+18-1.000  0.000  1000.0  2000.0

 1H     + 1H     + 1H2   = 1H2    + 1H2
Forward Rate Parameters:
Glarborg, et al. 1986                   9.2E+16-0.600  0.000  1000.0  2000.0
Warnatz, J. 1984                        9.7E+16-0.600  0.000   300.0  3000.0
Westbrook and Dryer                     3.0E+15 0.000  0.000   300.0   300.0

 1H     + 1H     + 1H2O  = 1H2    + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1986                   6.0E+19-1.250  0.000  1000.0  2000.0

 1H     + 1H     + 1CO2  = 1H2    + 1CO2
Forward Rate Parameters:
Glarborg, et al. 1986                   5.5E+20-2.000  0.000  1000.0  2000.0

 1H     + 1O2            = 1HO    + 1O
Forward Rate Parameters:
Glarborg, et al. 1986                   5.1E+16-0.820 16.510  1000.0  2000.0
Glarborg, et al. 1985
Westbrook and Dryer
Seeker, et al. 1985                     4.5E+18-1.000 14.805  1000.0  2000.0
Warnatz, J. 1984                        1.2E+17-0.910 16.520   300.0  2500.0
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*----------------------------------------------------------------------*
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*----------------------------------------------------------------------*


 1H    + 1O2   + 1M    = 1HO2  + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                       2.1E+18-1.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                         1.5E+15 0.000 -1.000   300.0  2000.0
Seeker, et al. 1985                         1.0E+15 0.000 -1.000  1000.0  2000.0
Warnatz, J. 1984                            7.0E+17-0.800  0.000   300.0  2000.0

 1H    + 1O2   + 1H2   = 1HO2  + 1H2
Forward Rate Parameters:
Warnatz, J. 1984                            2.0E+18-0.800  0.000   300.0  2500.0

 1H    + 1O2   + 1O2   = 1HO2  + 1O2
Forward Rate Parameters:
Glarborg, et al. 1986                       6.7E+19-1.420  0.000  1000.0  2000.0
Reverse Rate Parameters:
Glarborg, et al. 1985                       1.3E+20 1.460 46.790  1000.0  2000.0

 1H    + 1O2   + 1N2   = 1HO2  + 1N2
Forward Rate Parameters:
Glarborg, et al. 1986                       6.7E+19-1.420  0.000  1000.0  2000.0
Reverse Rate Parameters:
Glarborg, et al. 1985                       1.3E+20 1.460 46.790  1000.0  2000.0

 1HO   + 1HO           = 1H2O  + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                       6.0E+08 1.300  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                         2.1E+09 1.100  0.000  1000.0  2000.0
Reverse Rate Parameters:
Westbrook and Dryer                         6.8E+13 0.000 18.360   300.0  2000.0
Warnatz, J. 1984                            1.5E+10 1.140 17.260   300.0  2500.0

 1HO   + 1H    + 1M    = 1H2O  + 1M    +
Forward Rate Parameters:
Glarborg, et al. 1986                       7.5E+23-2.600  0.000  1000.0  2000.0
Westbrook and Dryer                         1.4E+23-2.000  0.000  1000.0  3000.0
Warnatz, J. 1984
Seeker, et al. 1985                         2.2E+22-2.000  0.000  1000.0  2000.0

 1HO2  + 1H            = 1H2   + 1O2
Forward Rate Parameters:
Glarborg, et al. 1985                       2.5E+13 0.000  0.700   300.0  1000.0
Glarborg, et al. 1986
Seeker, et al. 1985
Warnatz, J. 1984
Westbrook and Dryer

 1HO2  + 1H            = 1HO   + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                       2.5E+14 0.000  1.900   300.0   800.0
Glarborg, et al. 1986
Seeker, et al. 1985
Westbrook and Dryer
```

```
Warnatz, J. 1984                          1.5E+14 0.000  1.000   300.0  1000.0

 1HO2  + 1H          = 1H2O  + 1O
Forward Rate Parameters:
Westbrook and Dryer                       5.0E+13 0.000  1.000  1000.0  2000.0

 1HO2  + 1O          = 1HO   + 1O2
Forward Rate Parameters:
Glarborg, et al. 1985                     4.8E+13 0.000  1.000   300.0  1000.0
Glarborg, et al. 1986
Westbrook and Dryer                       5.0E+13 0.000  1.000   300.0  1000.0
Seeker, et al. 1985
Warnatz, J. 1984                          2.0E+13 0.000  0.000   300.0  1000.0

 1HO2  + 1HO         = 1H2O  + 1O2
Forward Rate Parameters:
Glarborg, et al. 1985                     5.0E+13 0.000  1.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985
Warnatz, J. 1984                          2.0E+13 0.000  0.000   300.0  2000.0

 1HO2  + 1HO2        = 1H2O2 + 1O2
Forward Rate Parameters:
Glarborg, et al. 1985                     2.0E+12 0.000  0.000   300.0  1200.0
Glarborg, et al. 1986
Seeker, et al. 1985
Warnatz, J. 1984
Westbrook and Dryer                       1.0E+13 0.000  1.000   300.0  1000.0

 1H2O2 + 1M          = 1HO   + 1HO   + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                     1.2E+17 0.000 45.500   700.0  1500.0
Glarborg, et al. 1986
Seeker, et al. 1985
Westbrook and Dryer
Warnatz, J. 1984
This work                                 1.29E33 -4.86 53.200  1000.0  2500.0

 1H2O2 + 1H          = 1HO2  + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                     1.7E+12 0.000  3.750   300.0   800.0
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, J. 1984
Reverse Rate Parameters:
Seeker, et al. 1985                       7.3E+11 0.000 18.680  1000.0  2000.0

 1H2O2 + 1H          = 1H2O  + 1HO
Forward Rate Parameters:
Westbrook and Dryer                       3.2E+14 0.000  8.940   400.0   800.0
Seeker, et al. 1985                       3.0E+14 0.000  9.000   300.0  1000.0
Warnatz, J. 1984                          1.0E+13 0.000  3.590   300.0  1000.0

 1H2O2 + 1HO         = 1H2O  + 1HO2
```

```
Forward Rate Parameters:
Glarborg, et al. 1985                   1.0E+13 0.000  1.800   300.0   800.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985                     1.0E+13 0.000  1.000   300.0  1000.0
Warnatz, J. 1984                        7.0E+12 0.000  1.430   300.0  1000.0

 1O    + 1O    + 1M    = 1O2   + 1M    +
Forward Rate Parameters:
Westbrook and Dryer                     1.9E+13 0.000 -1.790   300.0  3000.0
Seeker, et al. 1985                     1.0E+18-1.000  0.000   300.0  3000.0
Warnatz, J. 1984                        1.0E+17-1.000  0.000   300.0  3000.0
Reverse Rate Parameters:
Glarborg, et al. 1985                   1.9E+11 0.500 95.560  1000.0  2000.0
Glarborg, et al. 1986

 1O    + 1H    + 1M    = 1HO   + 1M
Forward Rate Parameters:
Westbrook and Dryer                     1.0E+16 0.000  0.000  1000.0  2000.0

 1O    + 1HO   + 1M    = 1HO2  + 1M
Forward Rate Parameters:
Westbrook and Dryer                     1.0E+17 0.000  0.000  1000.0  2000.0

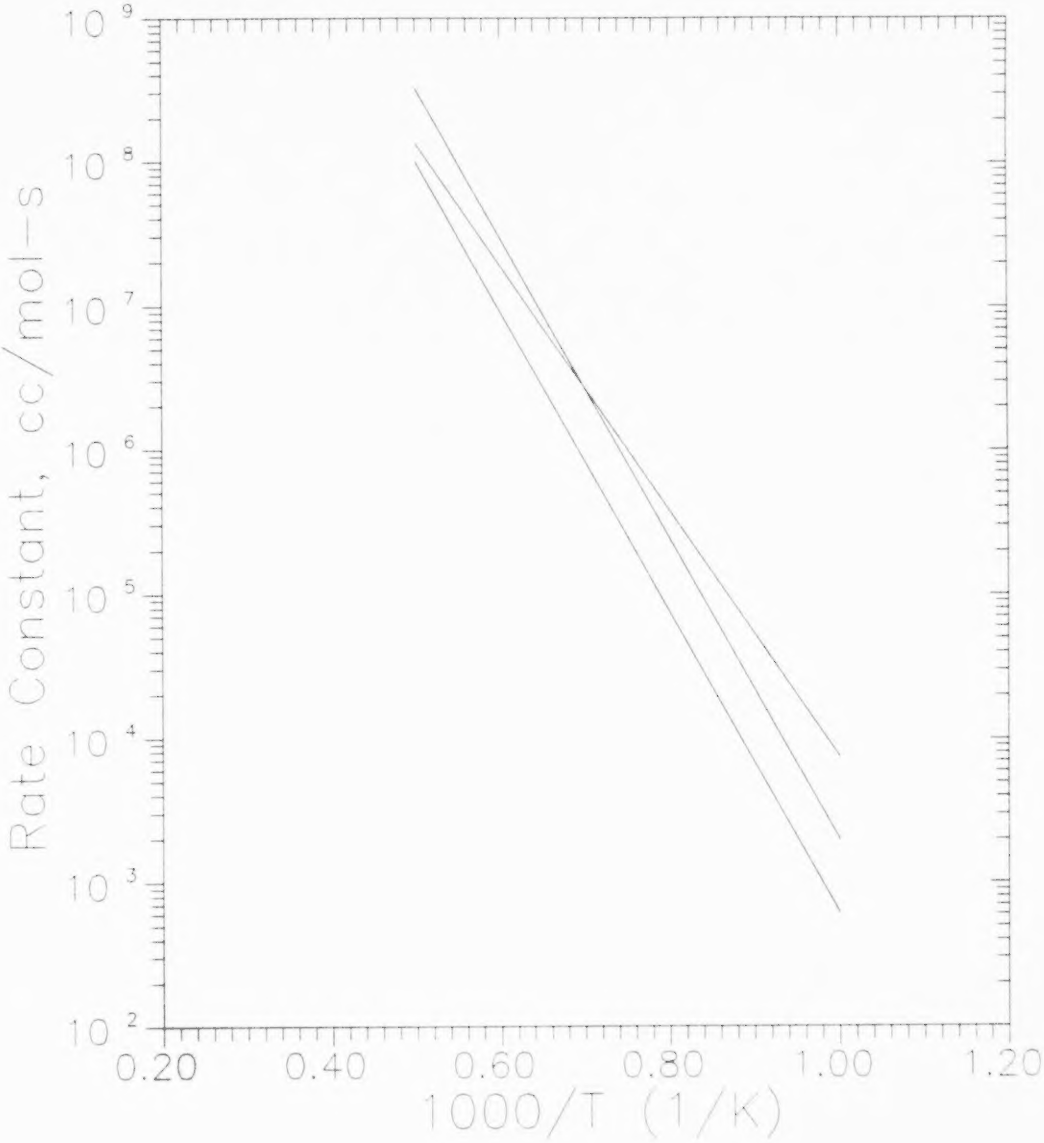
 1O    + 1HO           = 1HO2
Forward Rate Parameters:
Warnatz, J. 1984                        1.8E+13 0.000  0.000   300.0  2500.0

 1O3   + 1M            = 1O2   + 1O    + 1M
Forward Rate Parameters:
Westbrook and Dryer                     4.3E+14 0.000 22.180  1000.0  2000.0

 1O3   + 1O            = 1O2   + 1O2
Forward Rate Parameters:
Westbrook and Dryer                     1.1E+13 0.000  4.570  1000.0  2000.0

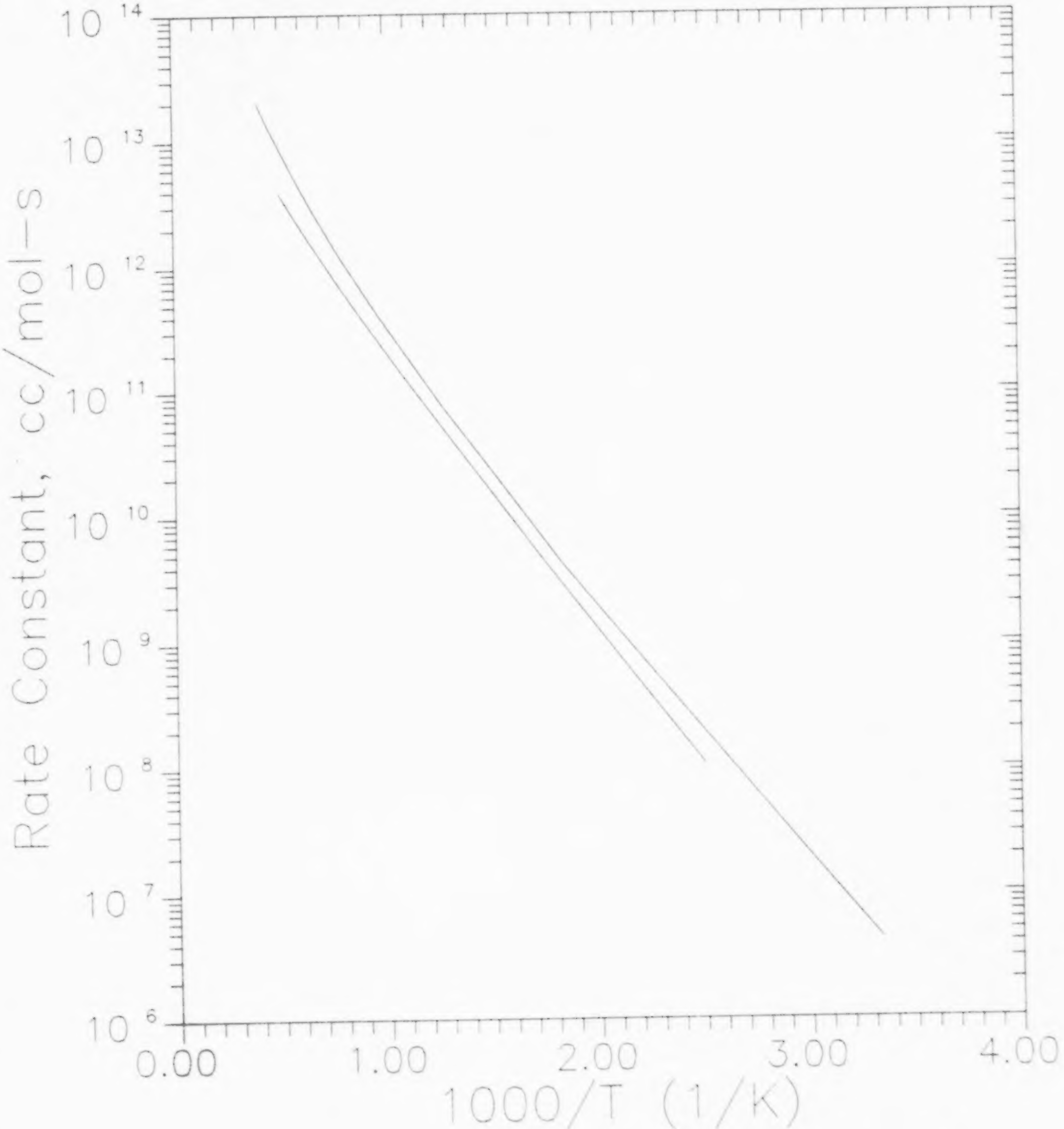
 1O3   + 1HO           = 1HO2  + 1O2
Forward Rate Parameters:
Westbrook and Dryer                     1.1E+12 0.000  1.848  1000.0  2000.0

 1O3   + 1H            = 1O2   + 1HO
Forward Rate Parameters:
Westbrook and Dryer                     7.9E+14 0.000  0.890  1000.0  2000.0
```

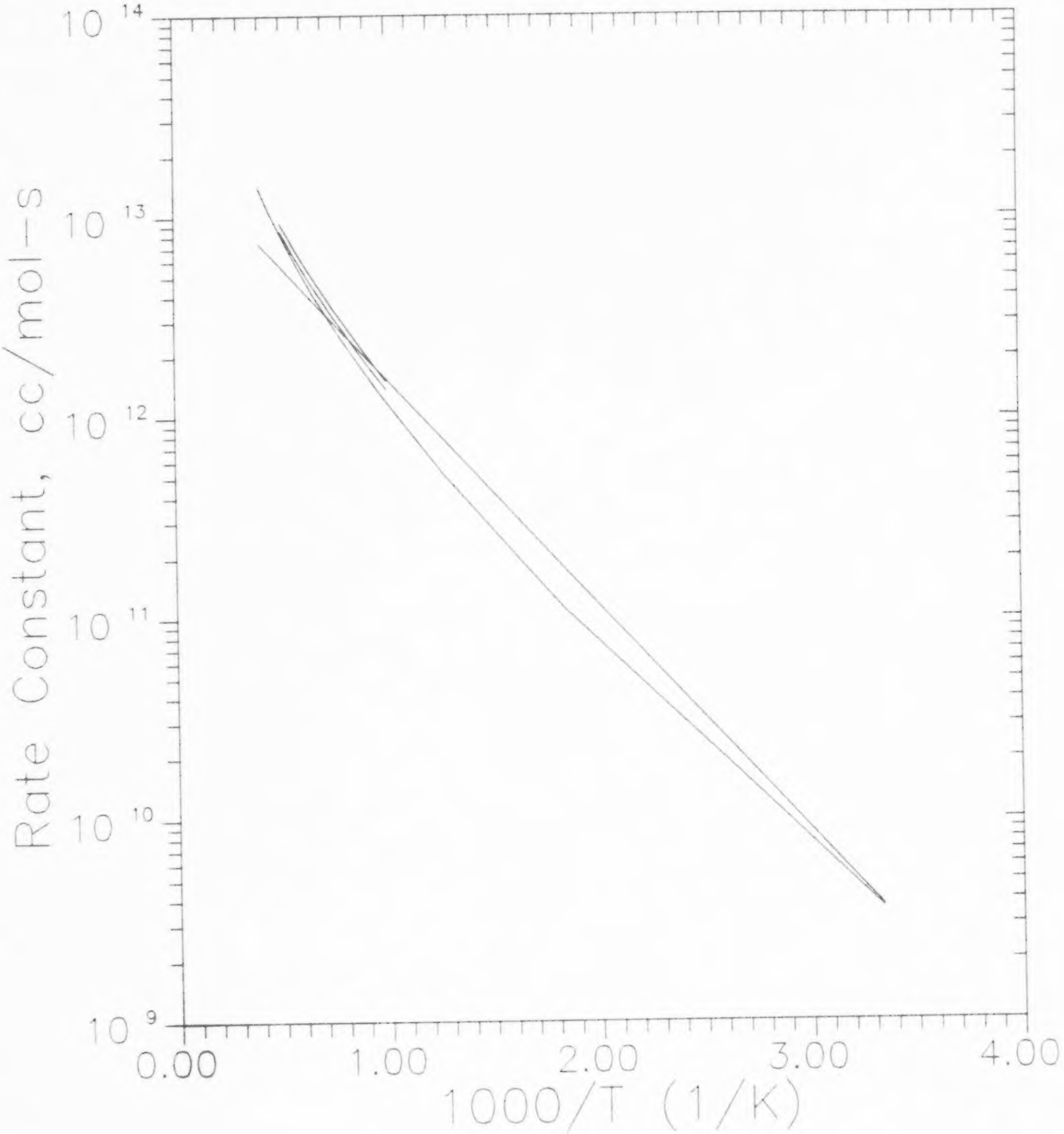


Rate Constant, cc/mol-s
$10^9$
$10^8$
$10^7$
$10^6$
$10^5$
$10^4$
$10^3$
$10^2$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**$H_2$ + $O_2$ = HO + HO**

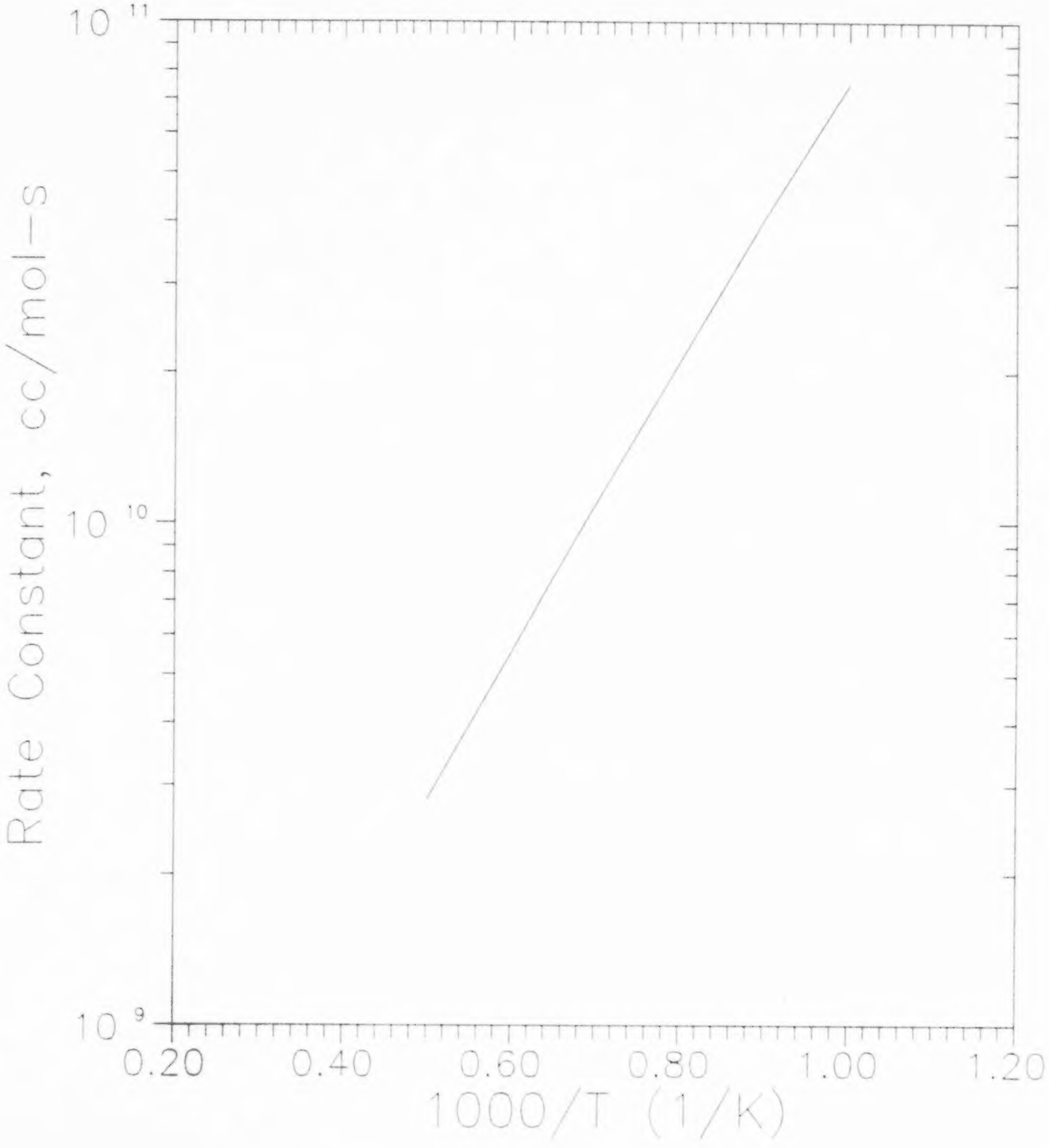

Rate Constant, cc/mol-s
10^14
10^13
10^12
10^11
10^10
10^9
10^8
10^7
10^6
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**H2 + O = HO + H**

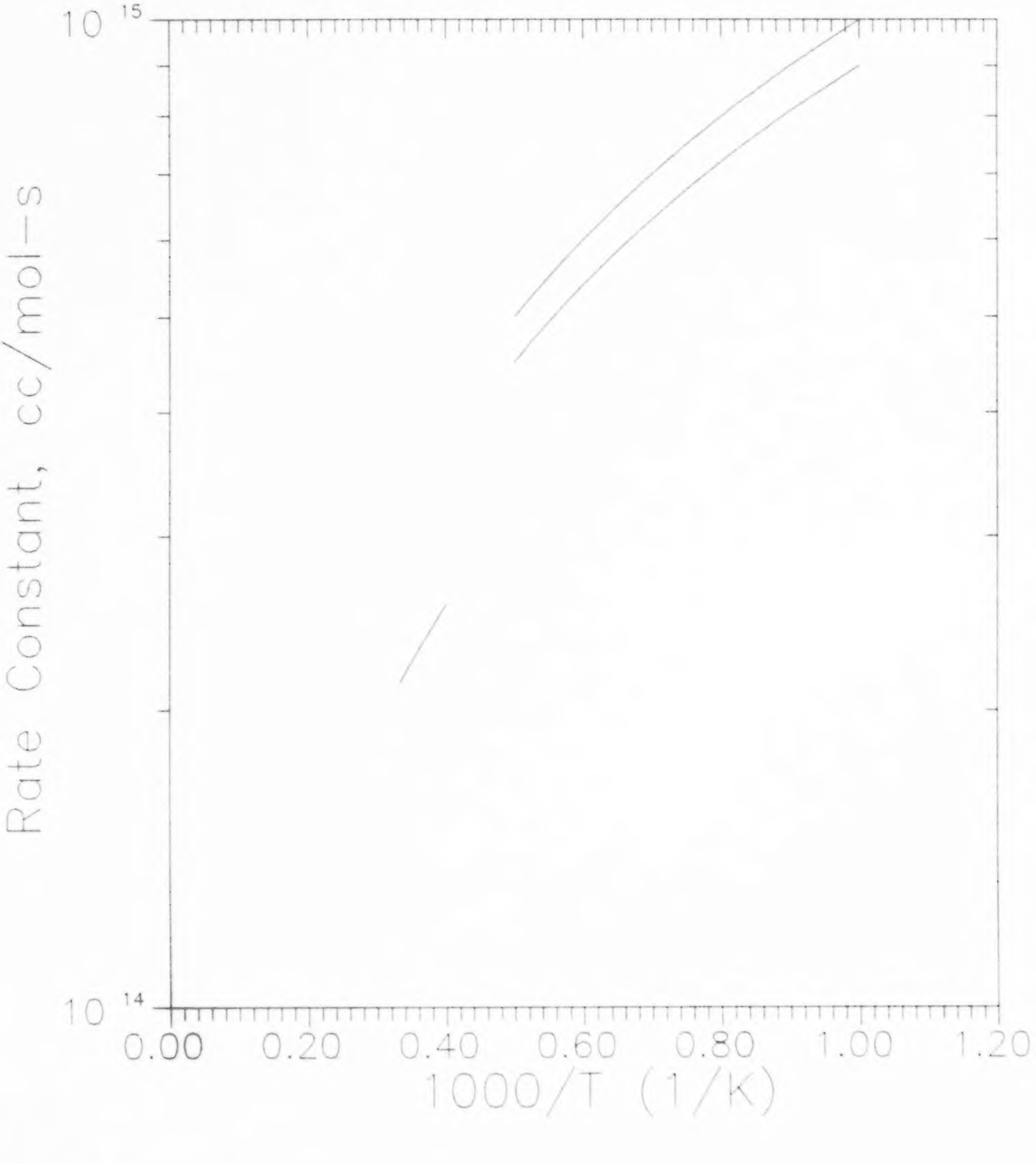


Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**$H_2$ + HO = $H_2O$ + H**

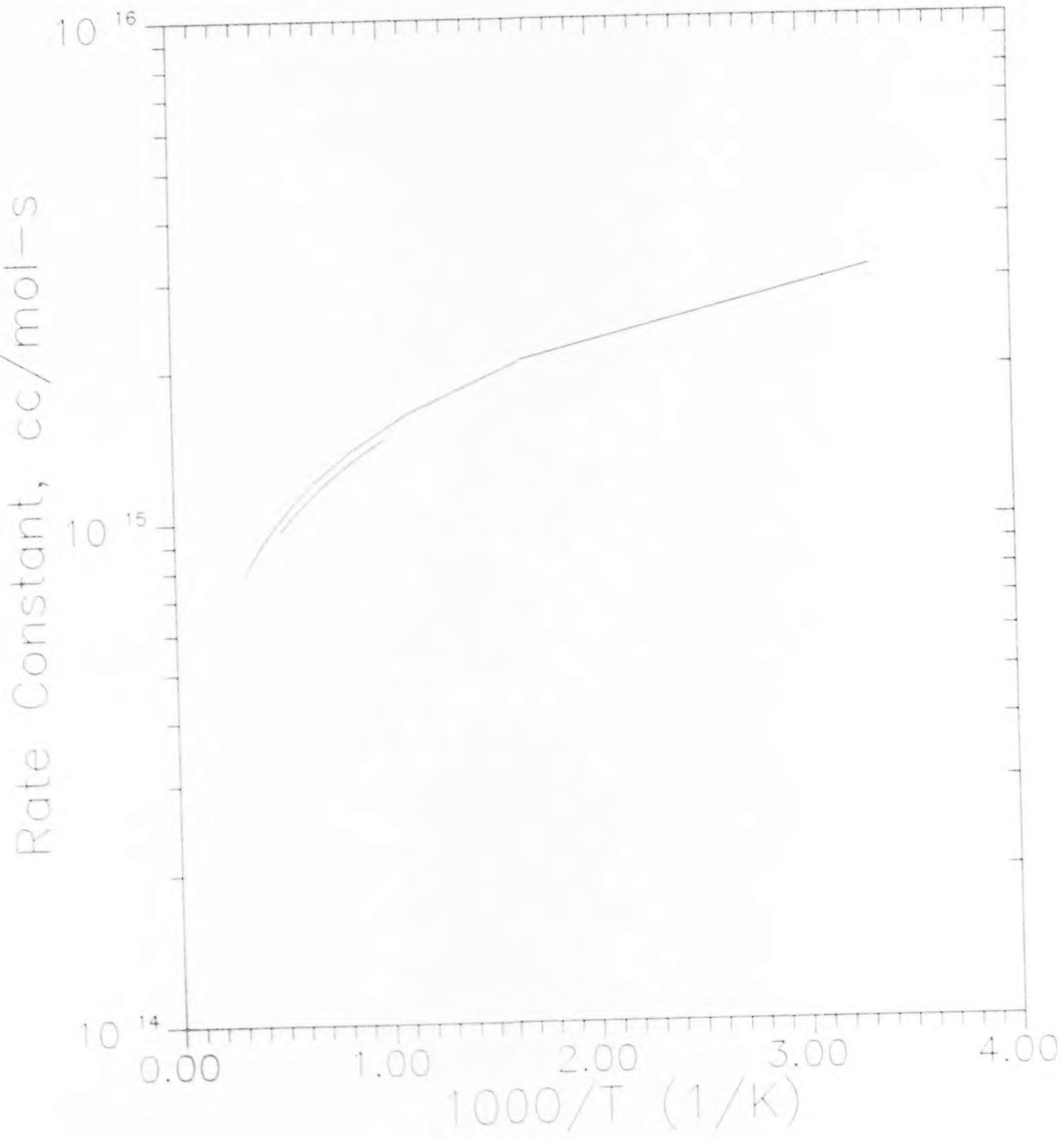

10 11
10 10
10 9
Rate Constant, cc/mol–s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**H + H + M = H2 + M**



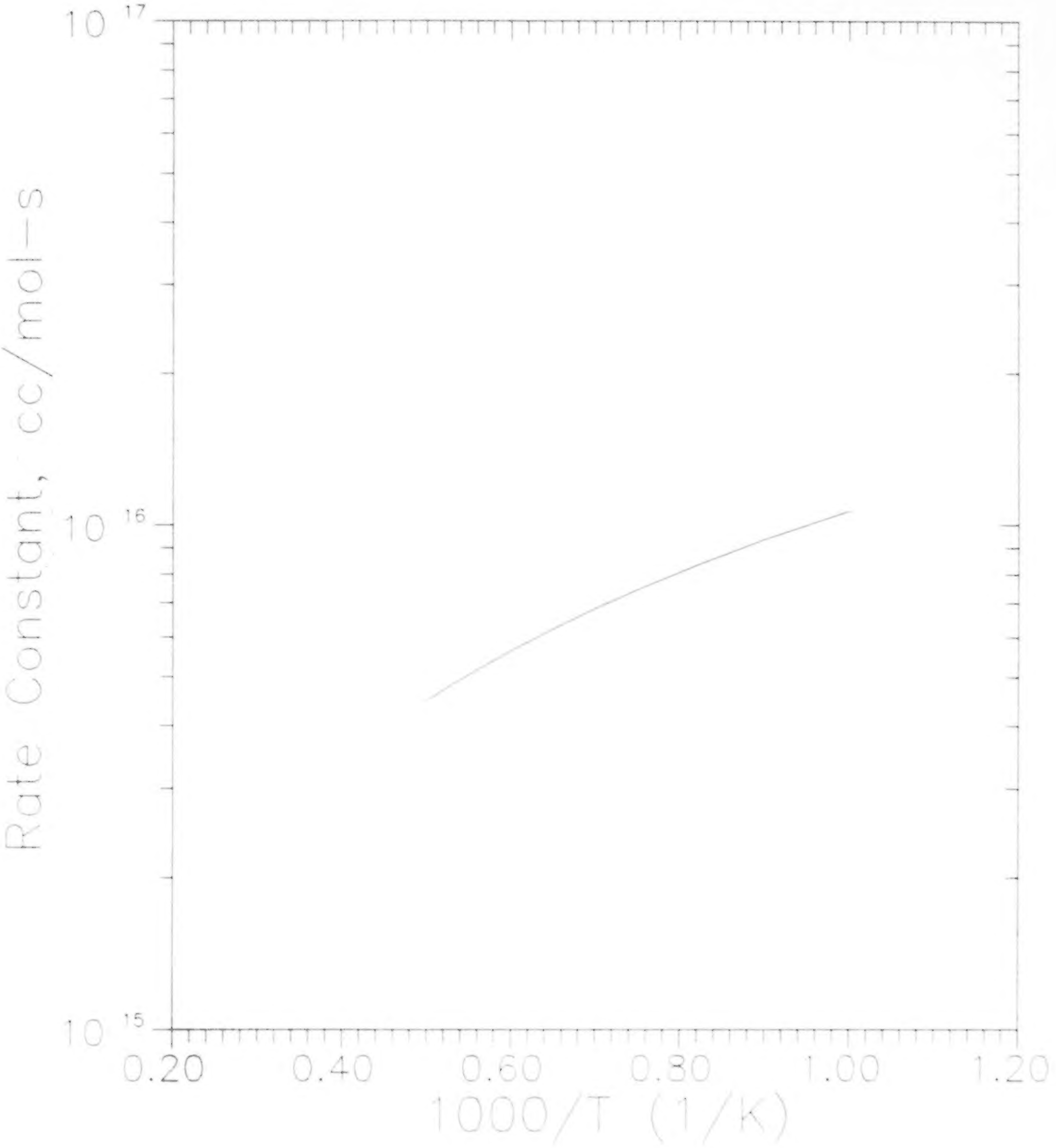
10 $^{15}$
10 $^{14}$
Rate Constant, cc/mol-s
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**H + H + AR = H2 + AR**



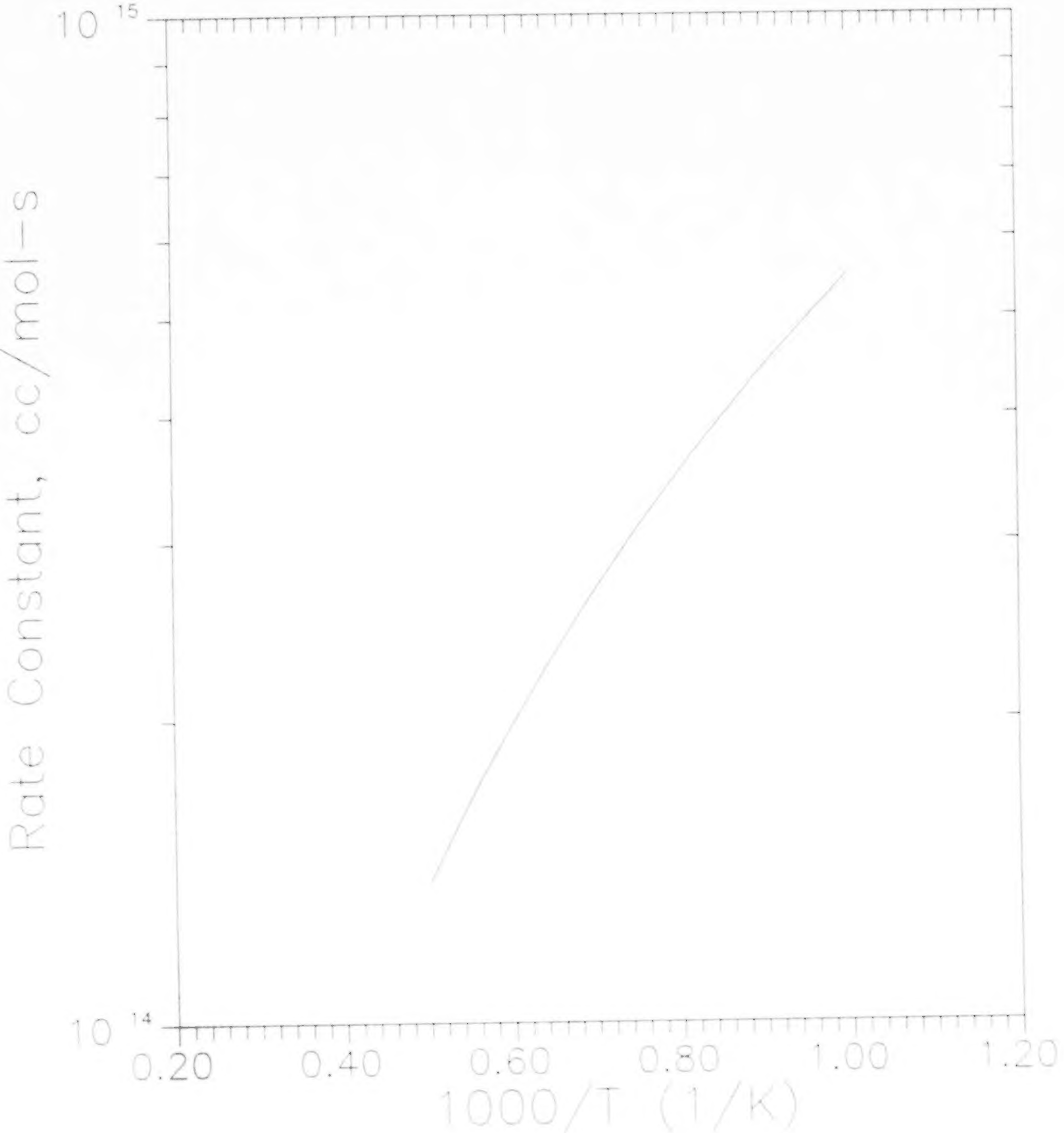
$10^{16}$
$10^{15}$
$10^{14}$
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**H + H + H2 = H2 + H2**

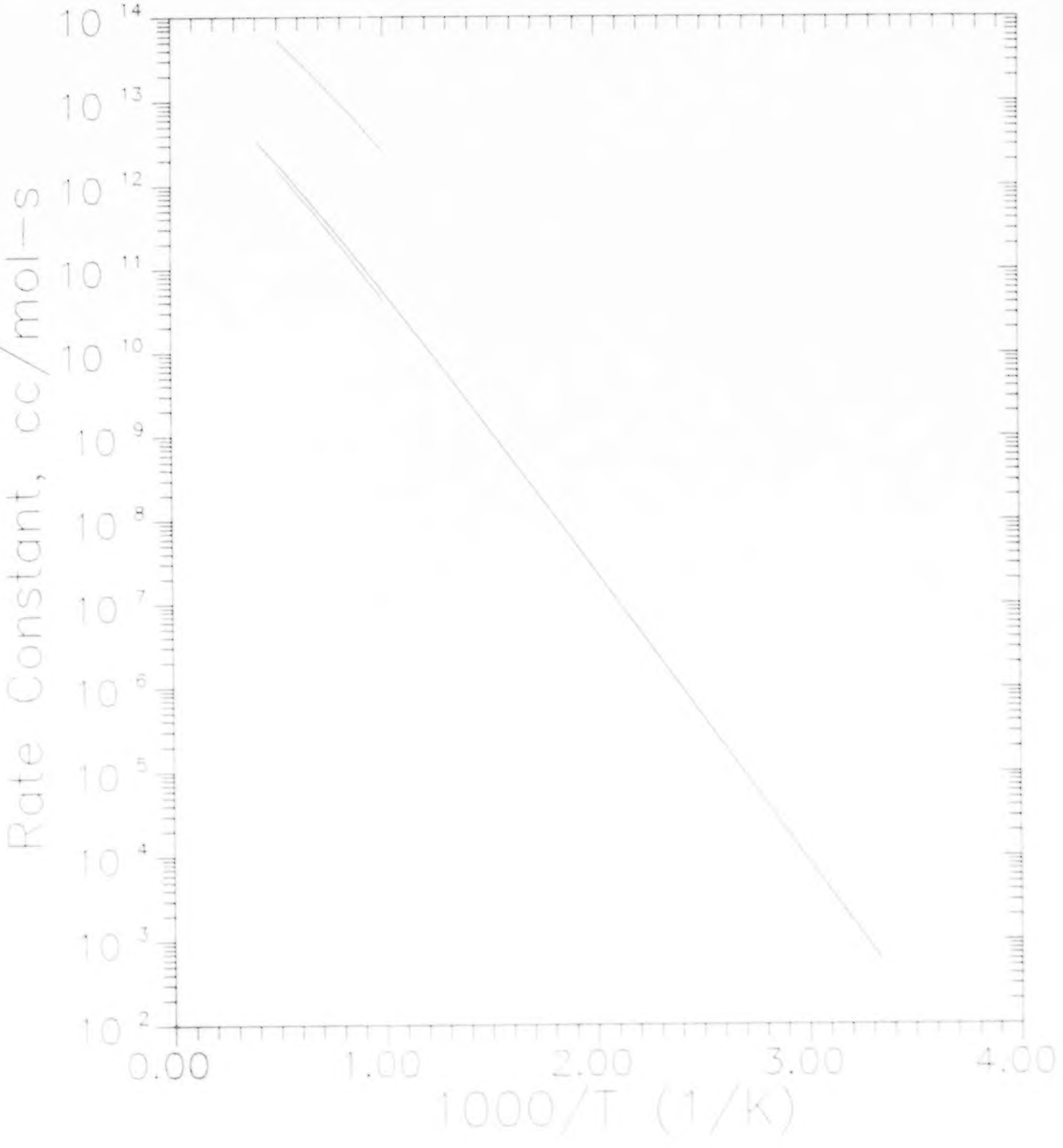


10 ^17
10 ^16
10 ^15
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

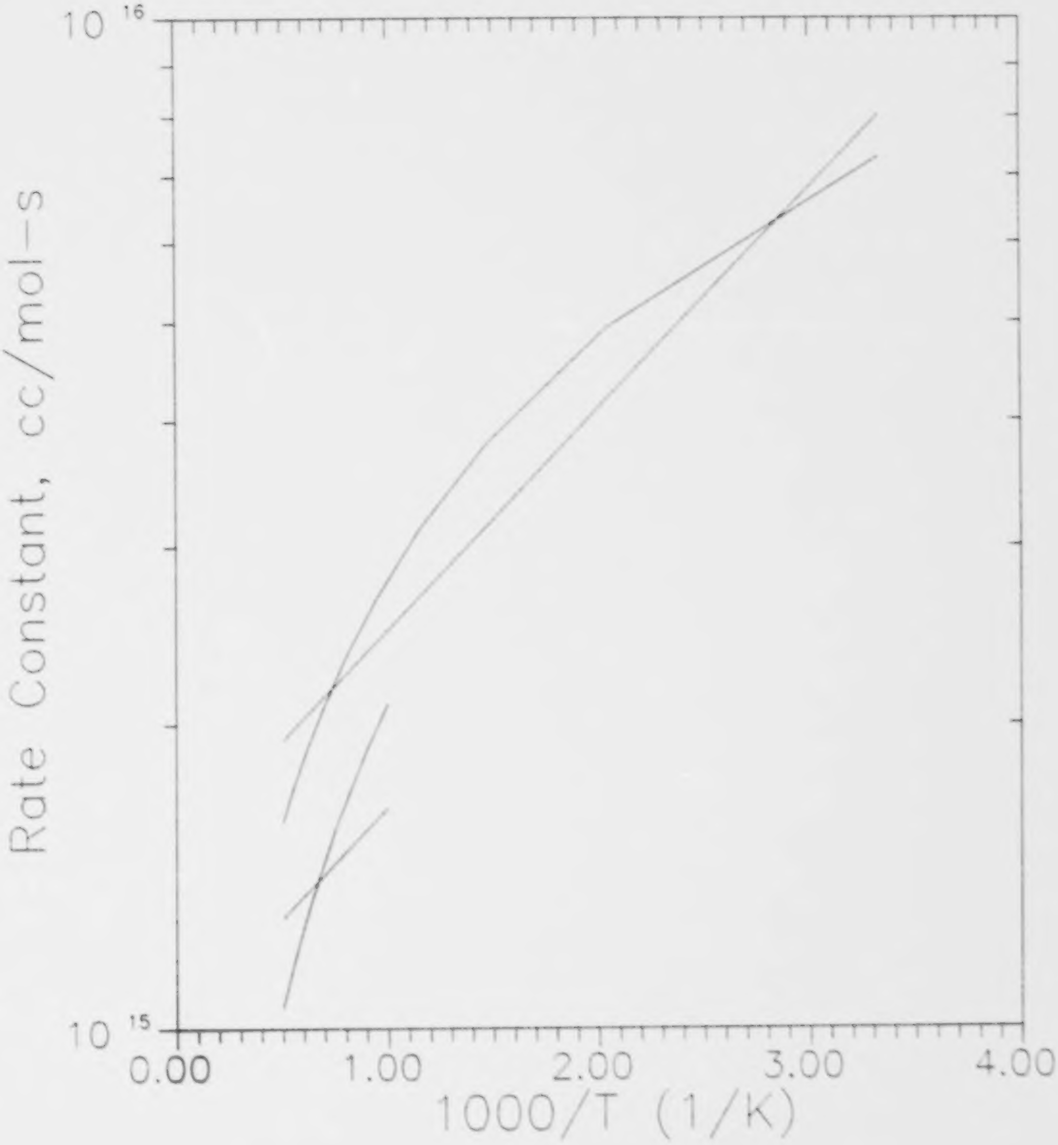
**H + H + H2O = H2 + H2O**


10 15
10 14
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

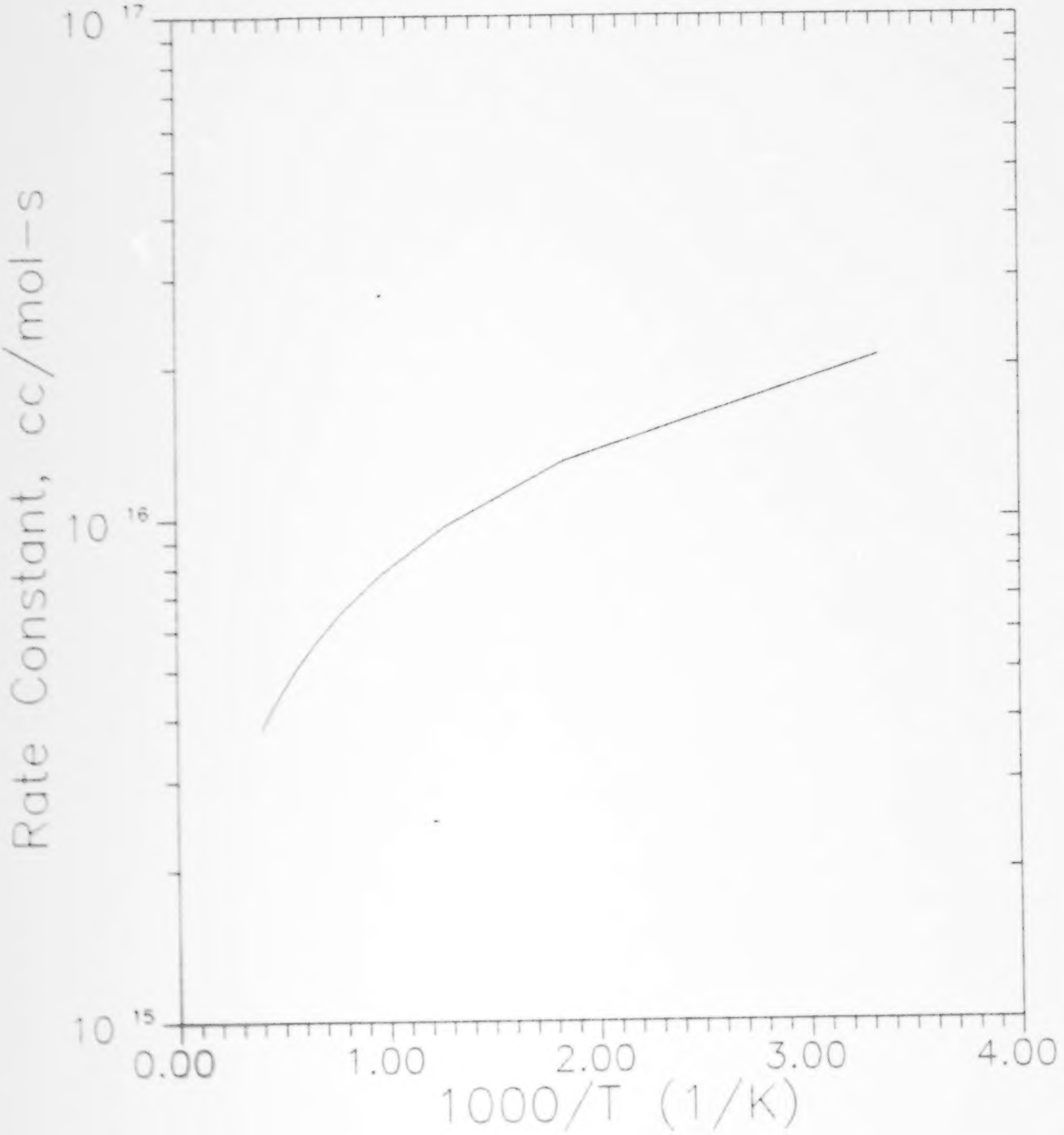
**H + H + CO2 = H2 + CO2**


Rate Constant, cc/mol-s
10 14
10 13
10 12
10 11
10 10
10 9
10 8
10 7
10 6
10 5
10 4
10 3
10 2
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

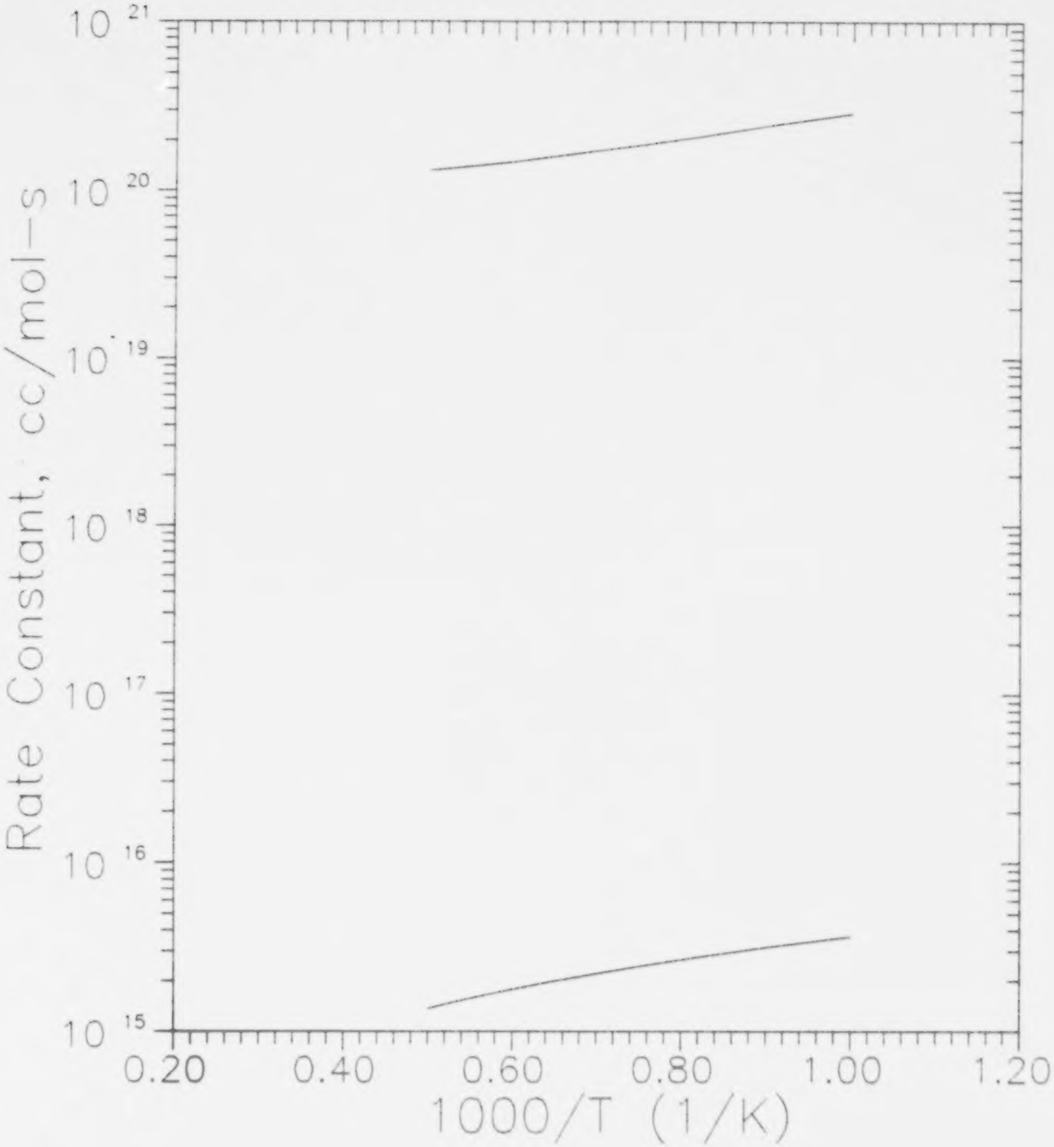
**H + O2 = HO + O**



**H + O2 + M = HO2 + M**

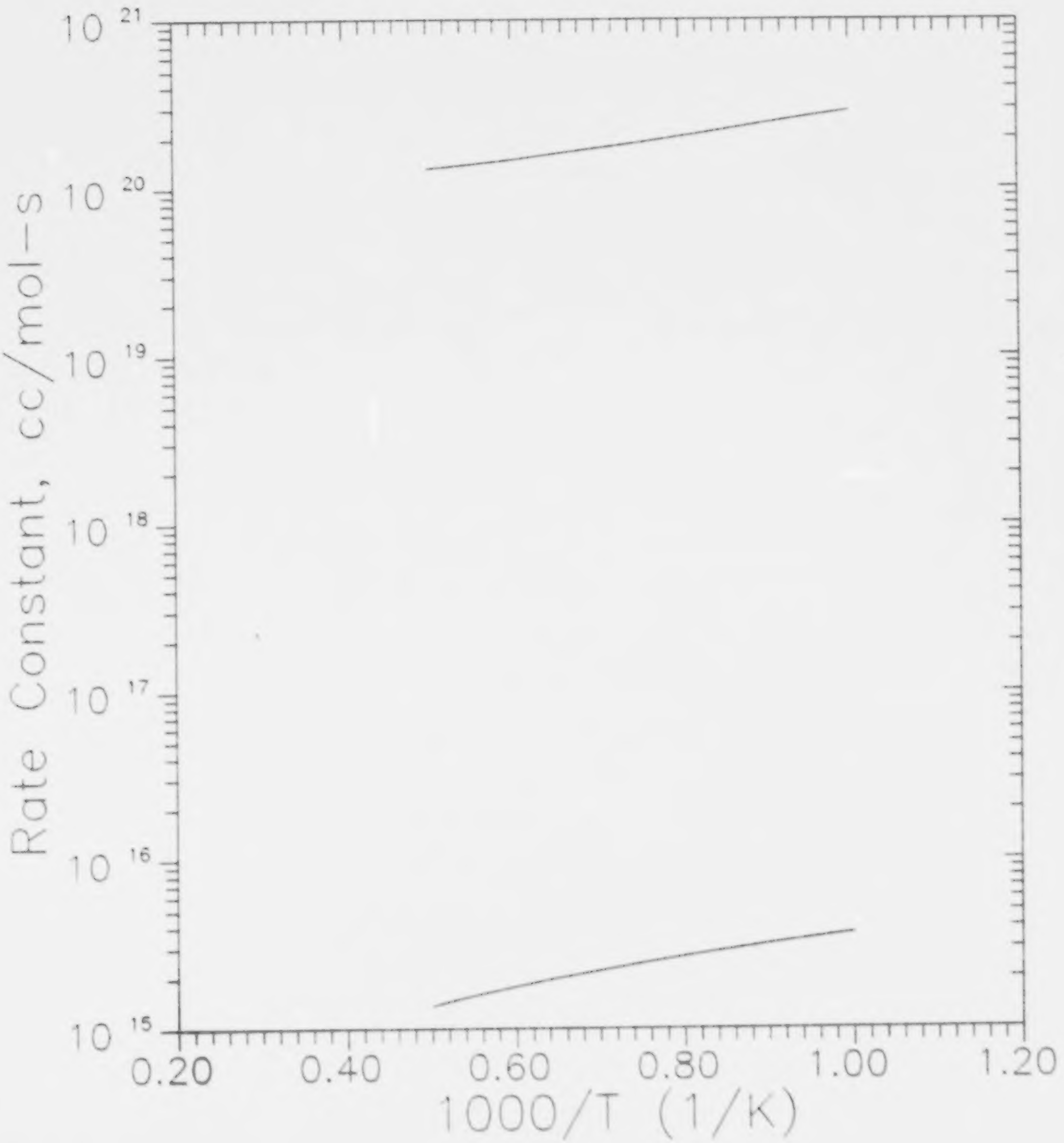

Rate Constant, cc/mol-s
$10^{17}$
$10^{16}$
$10^{15}$
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**H + O2 + H2 = HO2 + H2**

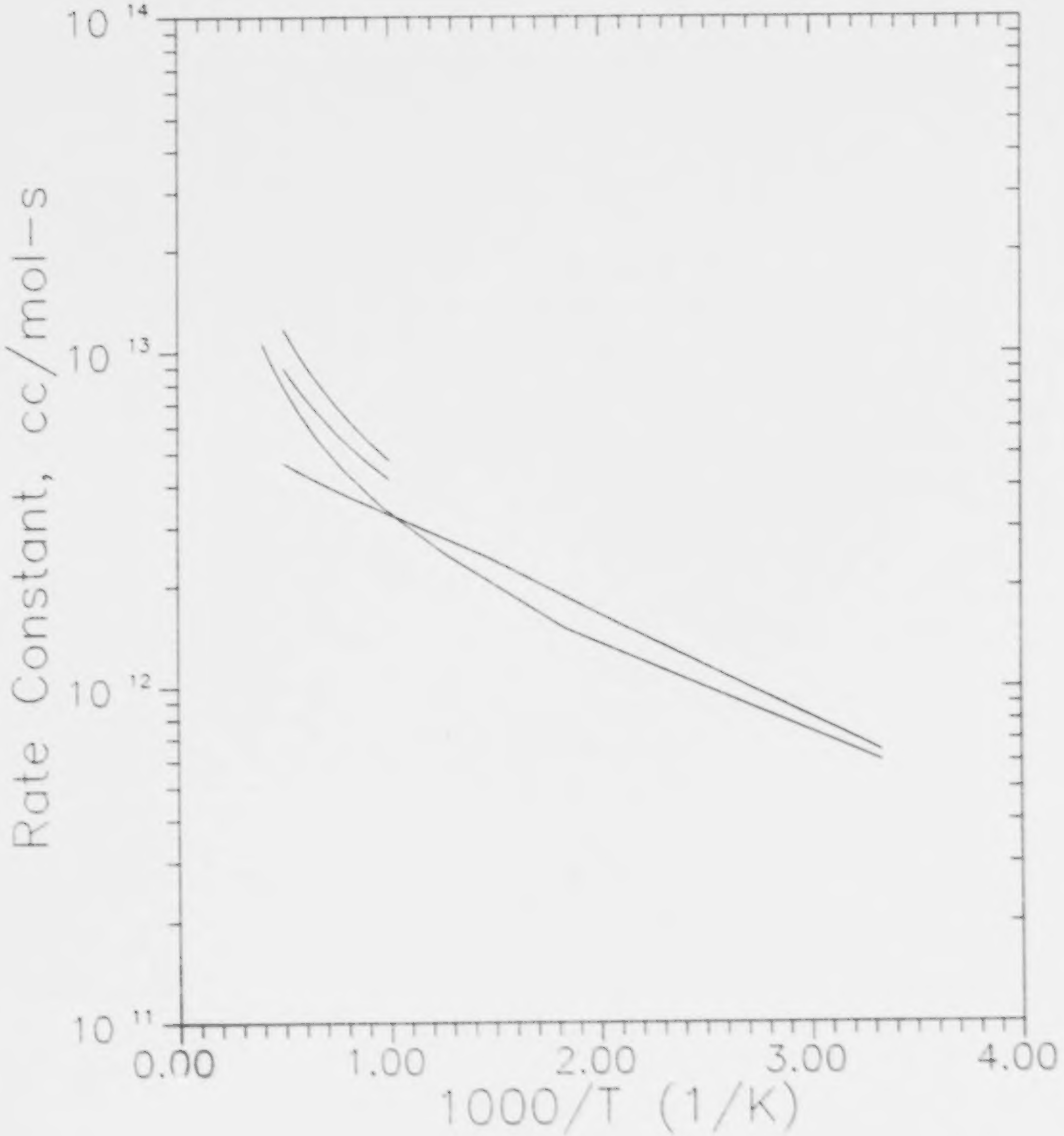


Rate Constant, cc/mol-s
10 21
10 20
10 19
10 18
10 17
10 16
10 15
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

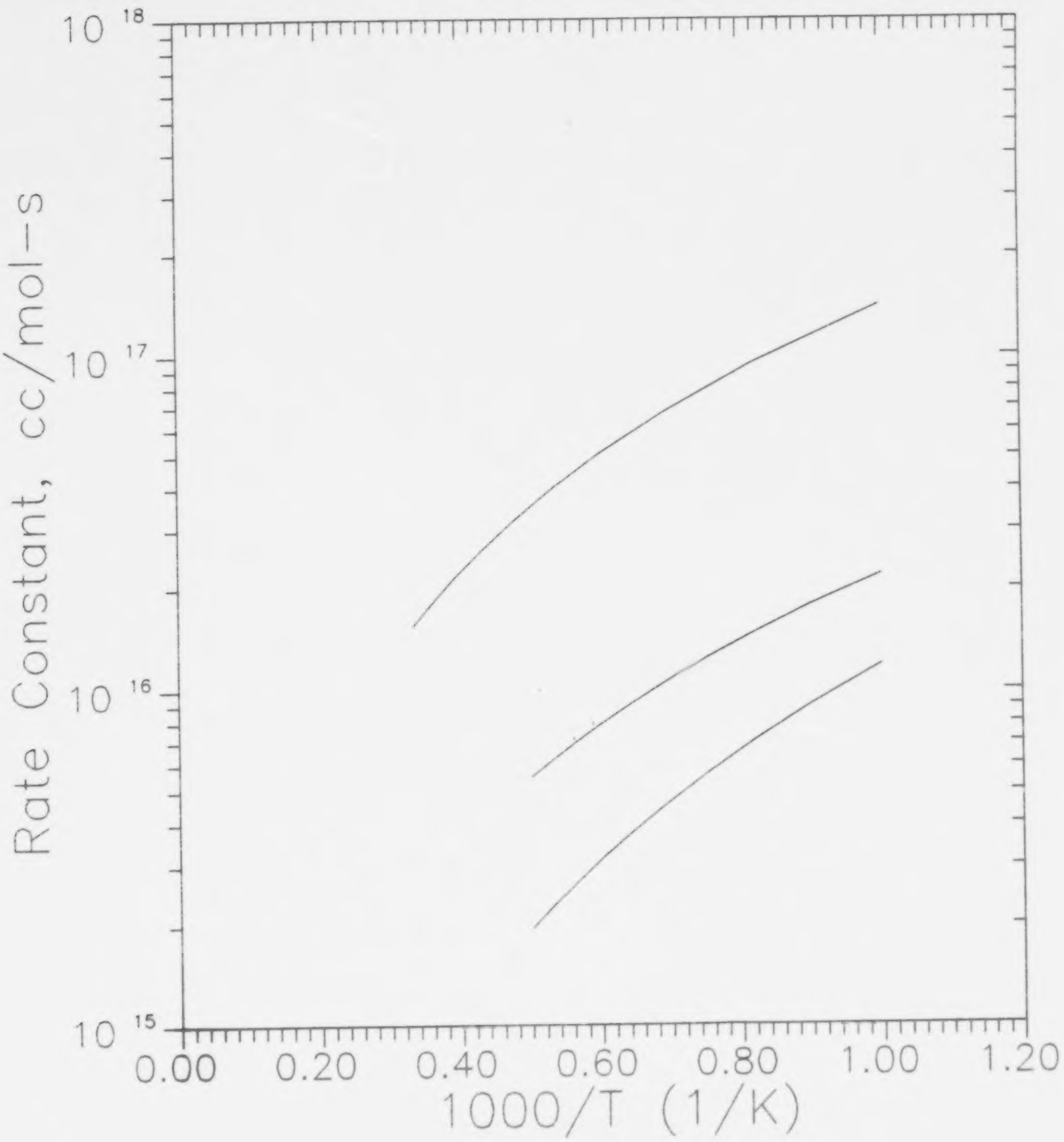
**H + O2 + O2 = HO2 + O2**


Rate Constant, cc/mol-s
10 21
10 20
10 19
10 18
10 17
10 16
10 15
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**H + O2 + N2 = HO2 + N2**

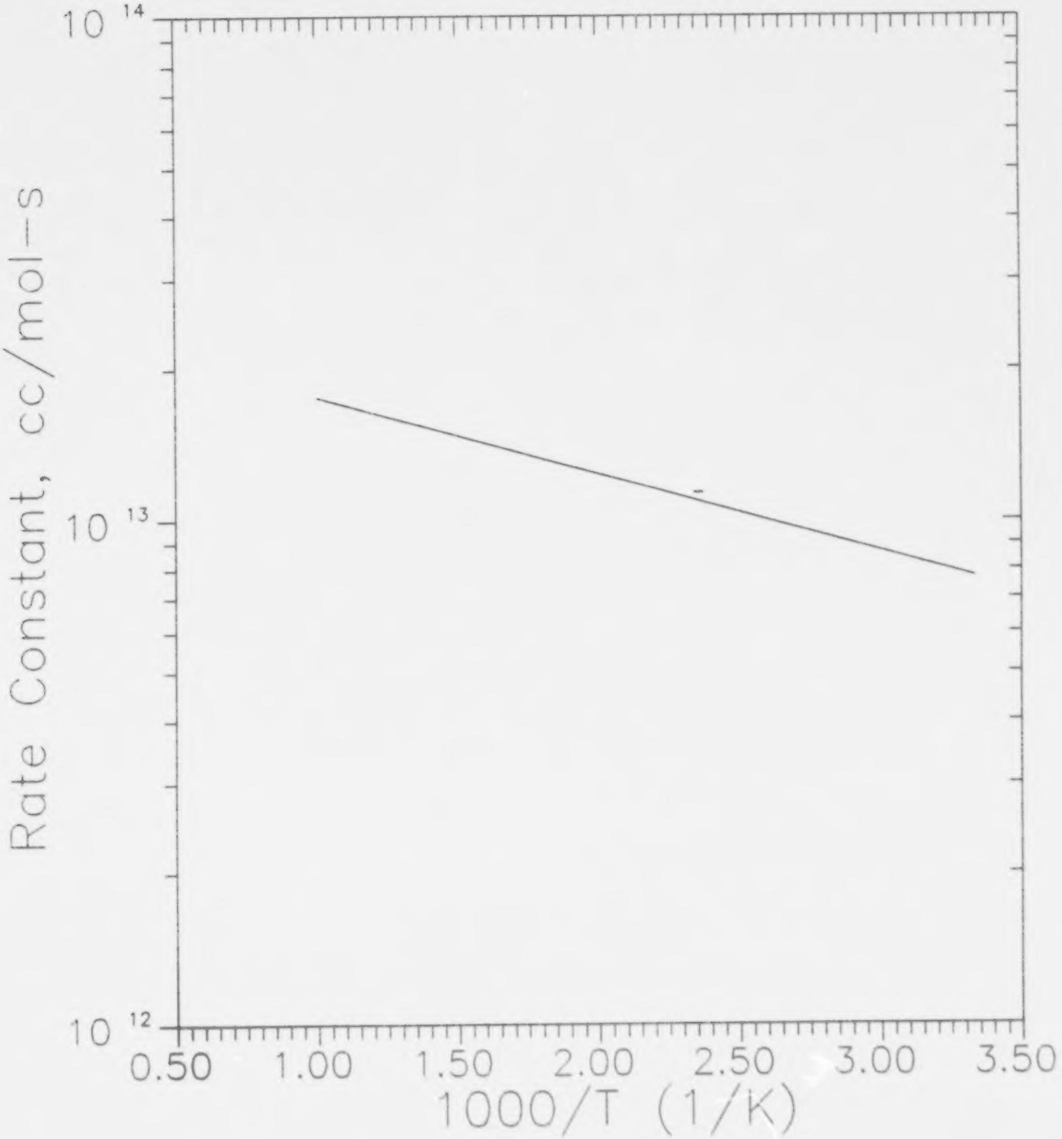

Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**HO + HO = H2O + O**



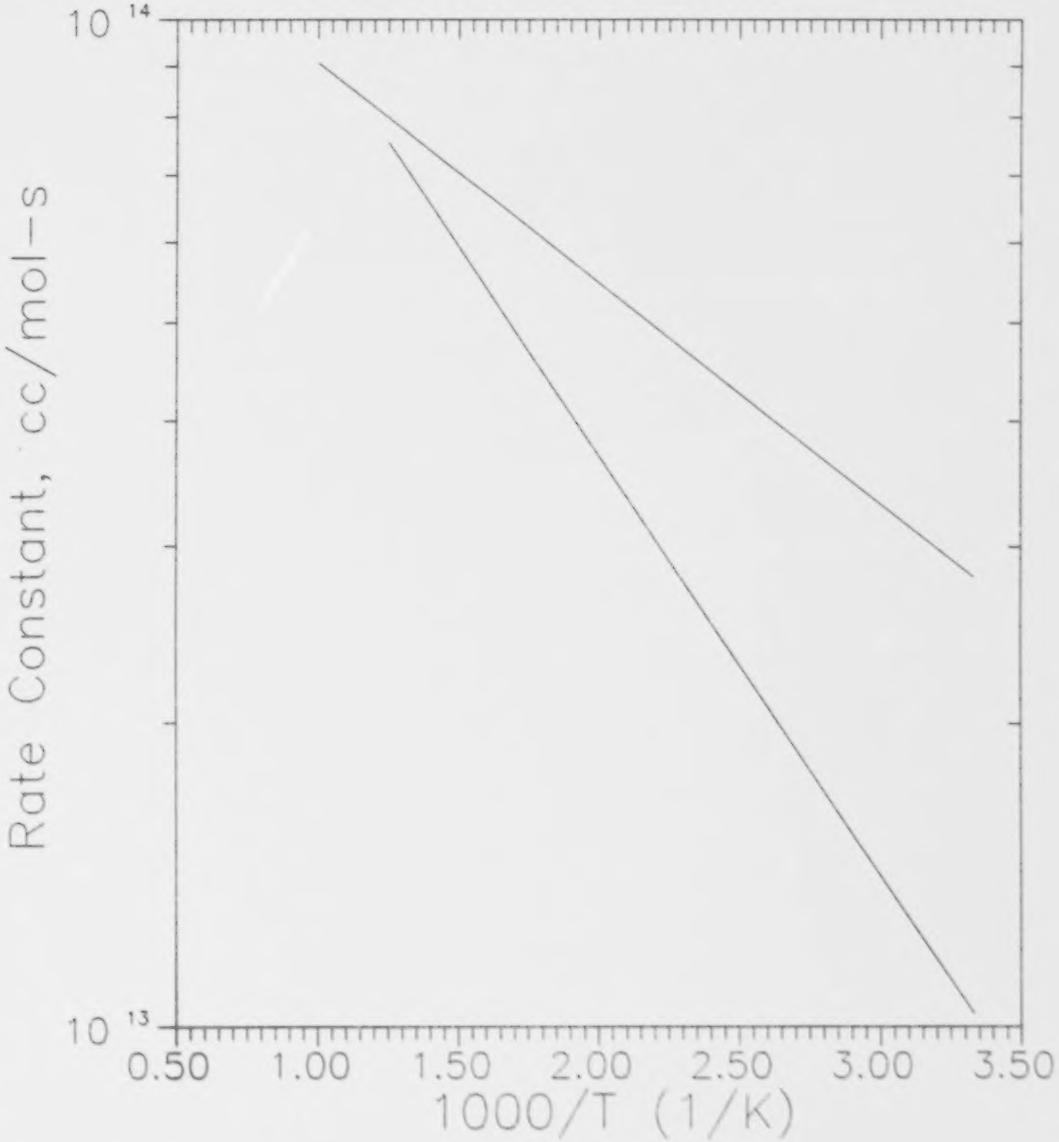
10^18
10^17
10^16
10^15
Rate Constant, cc/mol-s
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HO + H + M = H2O + M**



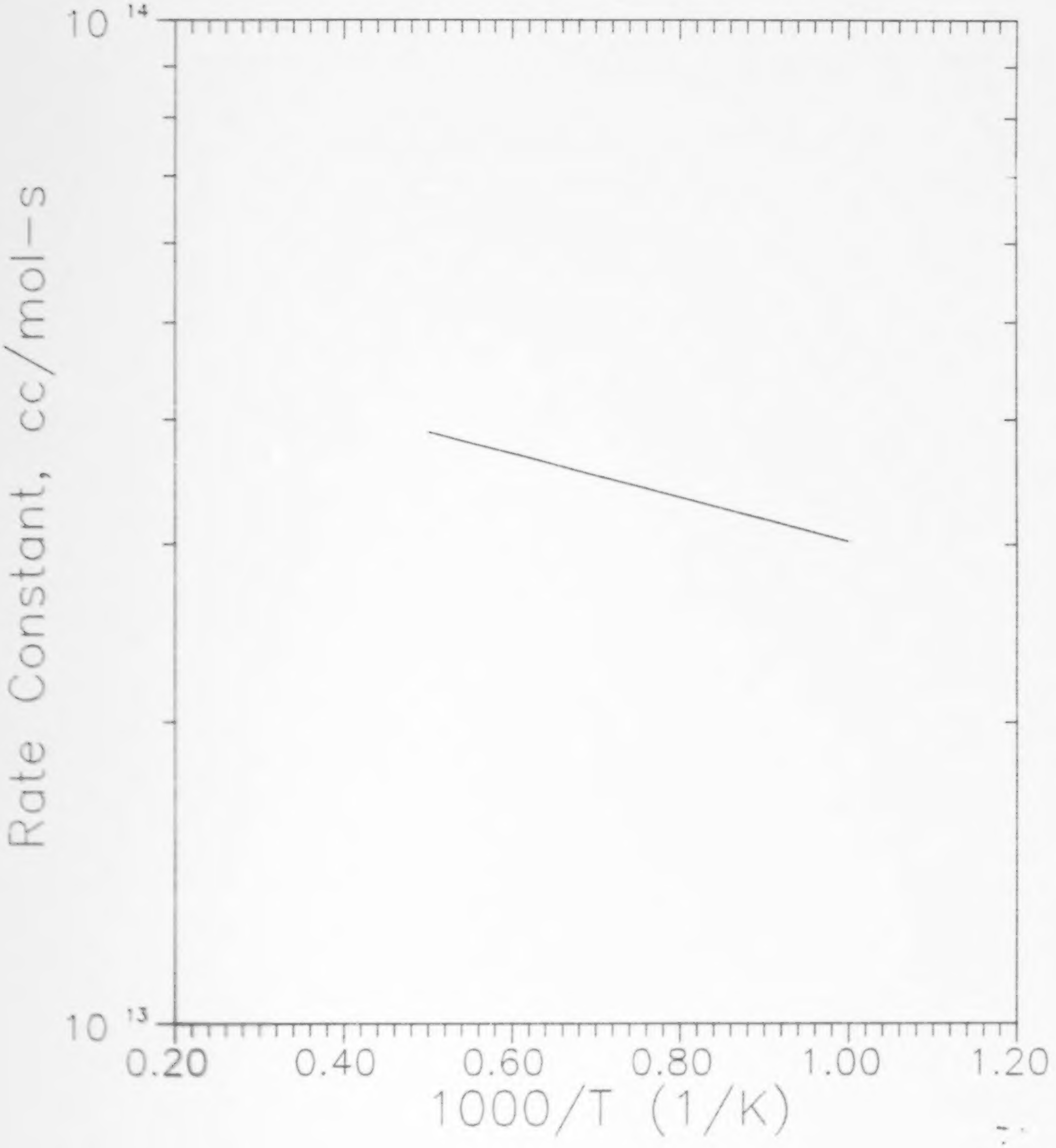
$10^{14}$
$10^{13}$
$10^{12}$
Rate Constant, cc/mol-s
0.50
1.00
1.50
2.00
2.50
3.00
3.50
1000/T (1/K)

**HO2 + H = H2 + O2**

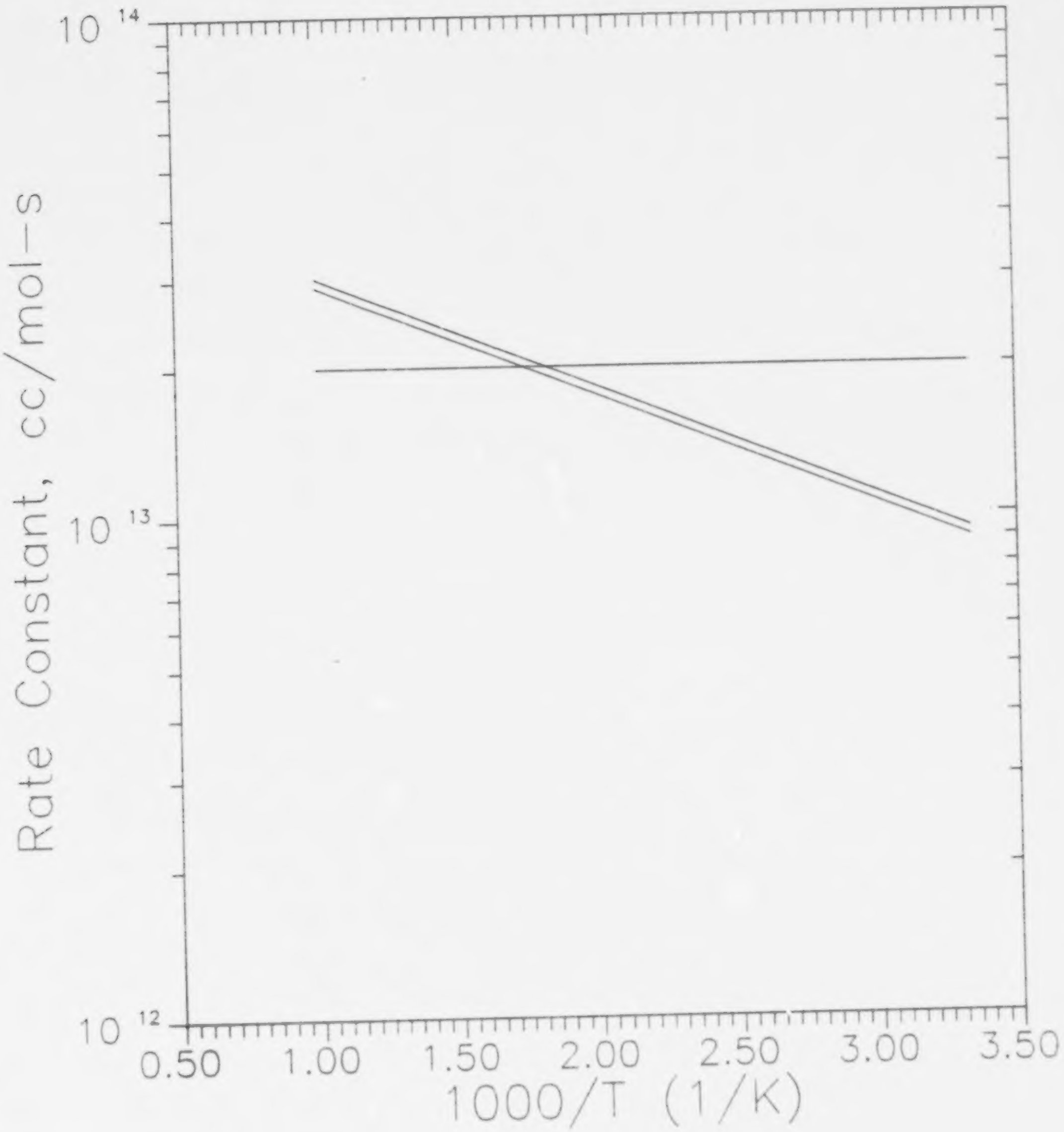


$10^{14}$
$10^{13}$
Rate Constant, cc/mol-s
0.50
1.00
1.50
2.00
2.50
3.00
3.50
1000/T (1/K)

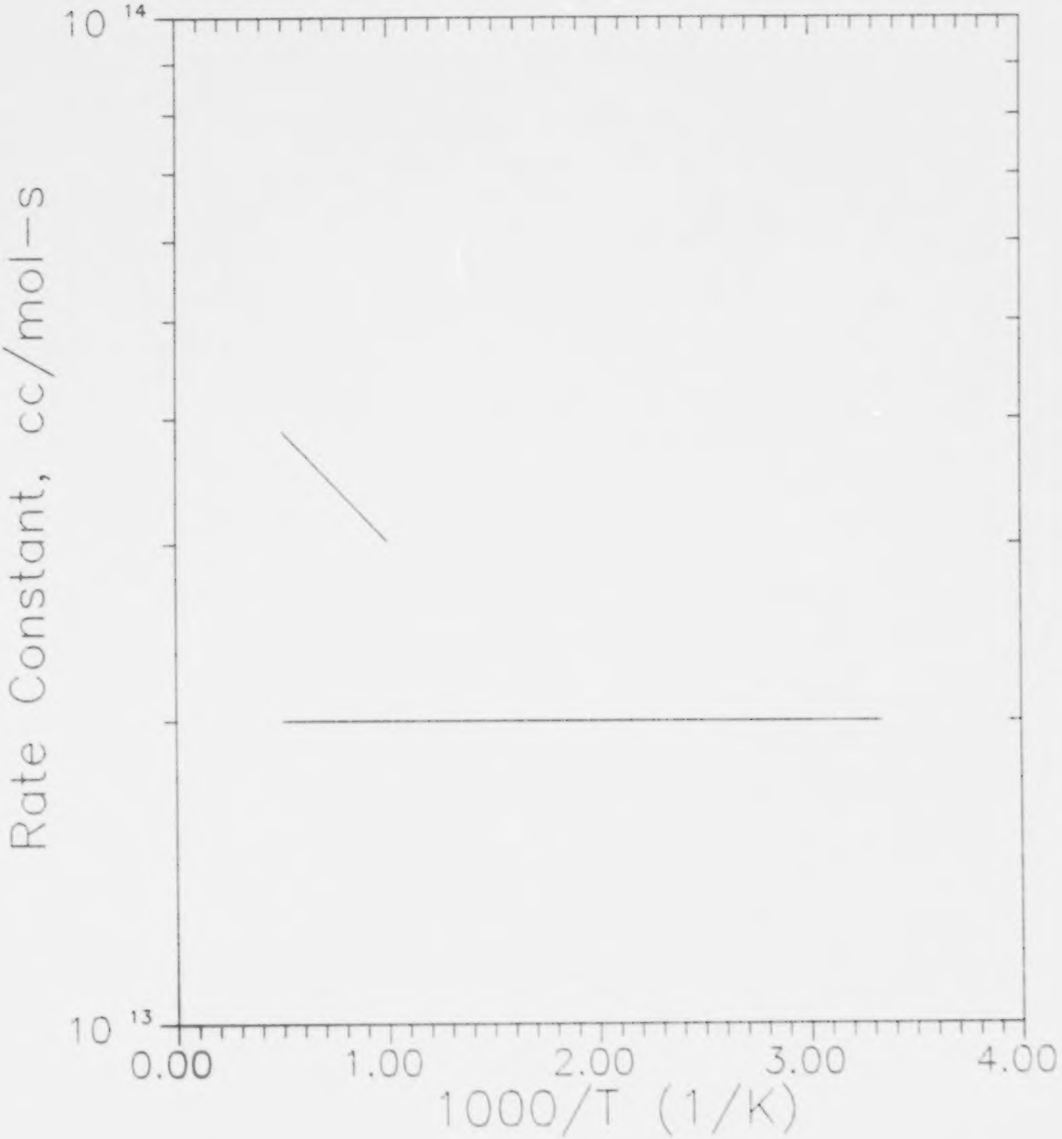
**HO2 + H = HO + HO**


10 ¹⁴
10 ¹³
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

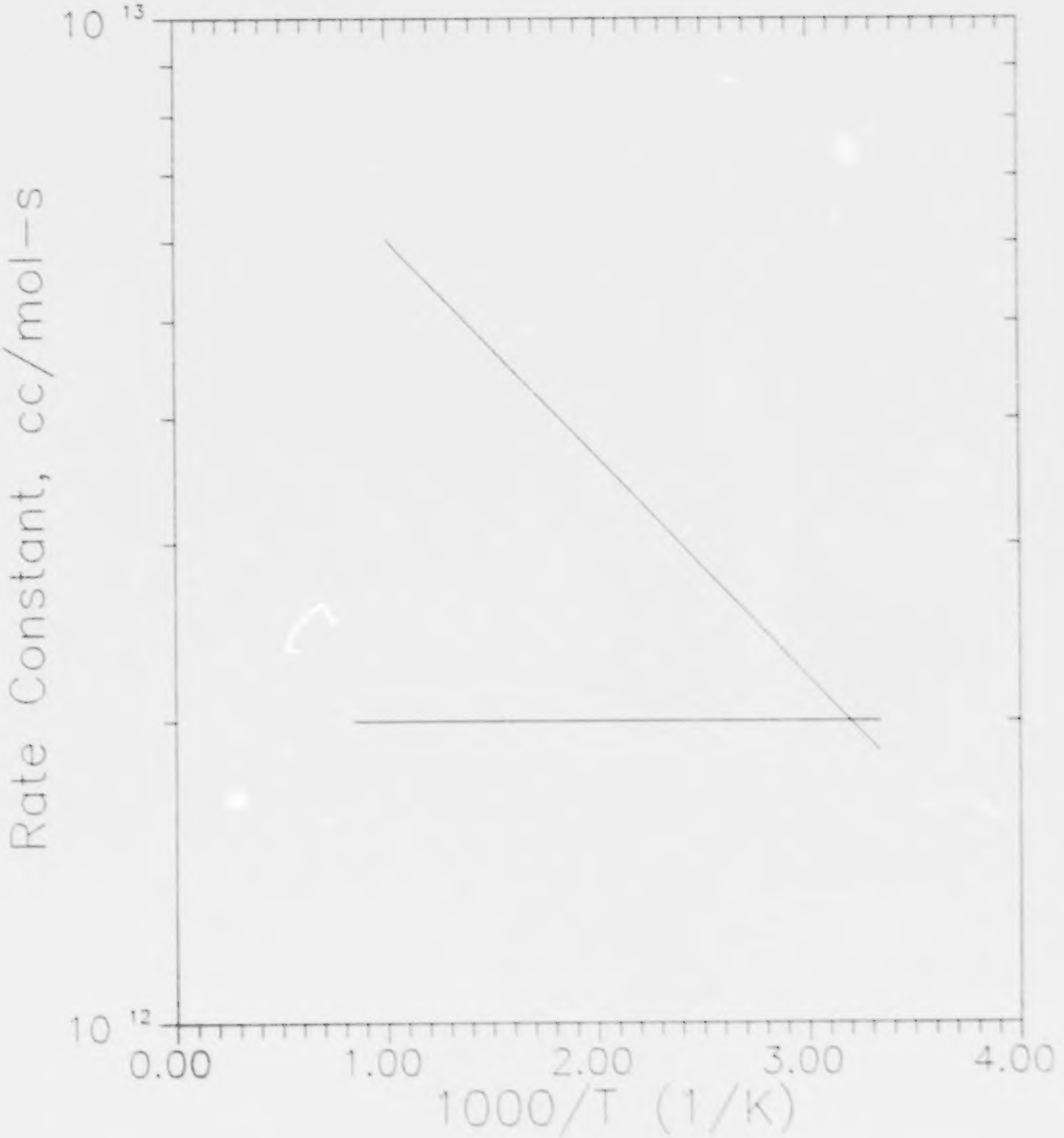
**$HO_2$ + H = $H_2O$ + O**


10 14
10 13
10 12
Rate Constant, cc/mol-s
0.50
1.00
1.50
2.00
2.50
3.00
3.50
1000/T (1/K)

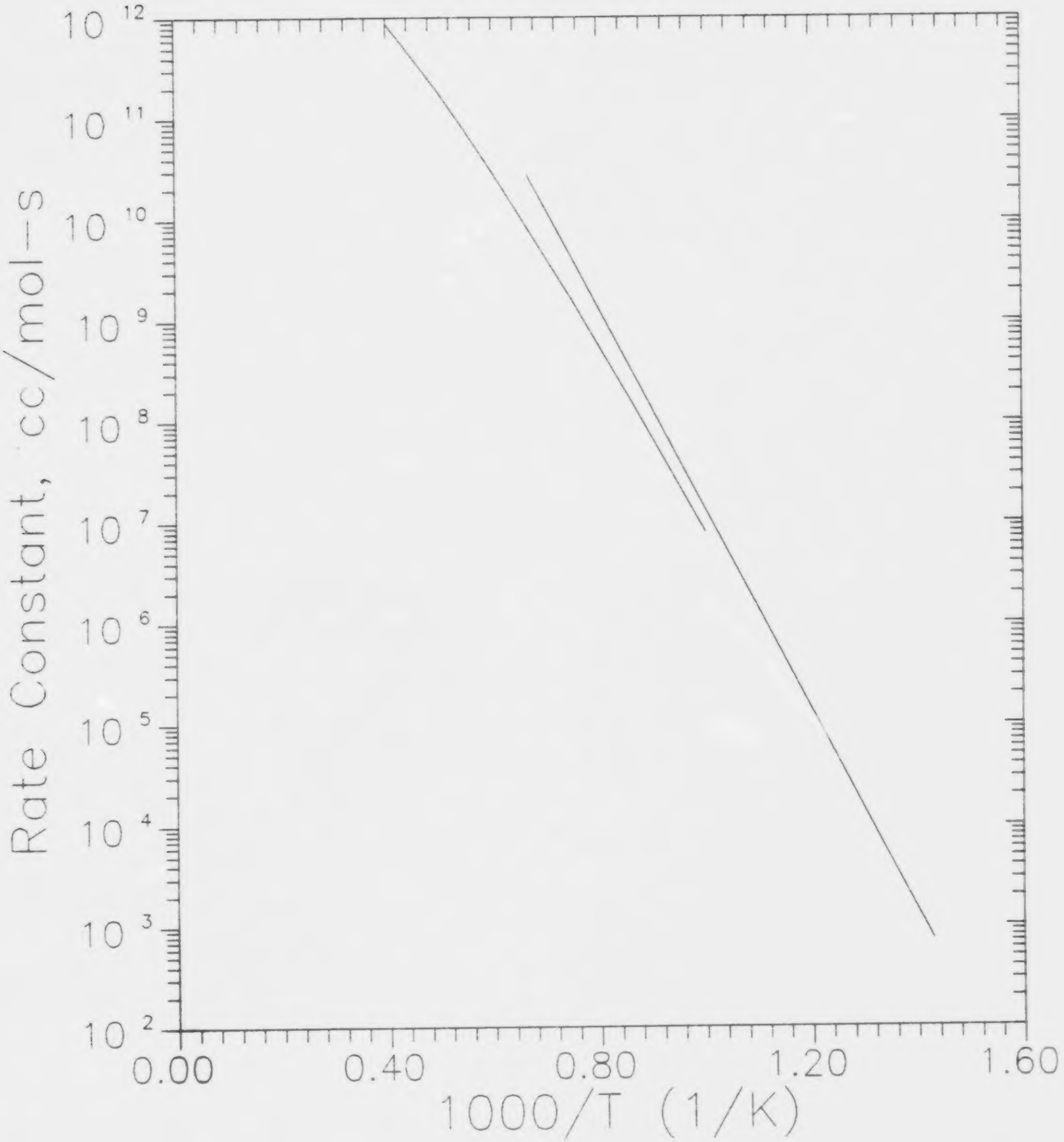
**HO2 + O = HO + O2**



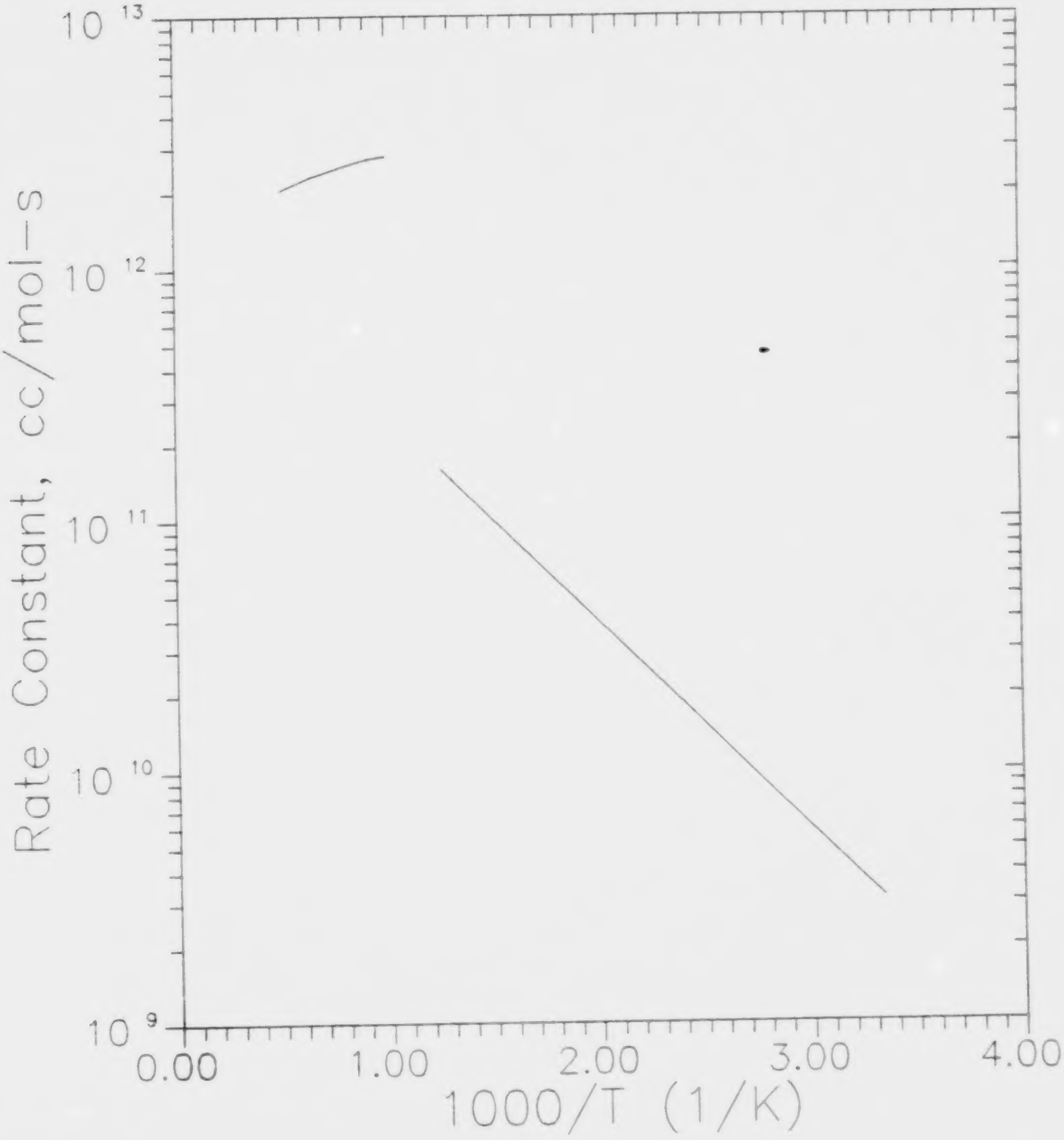
**HO2 + HO = H2O + O2**



**HO2 + HO2 = H2O2 + O2**

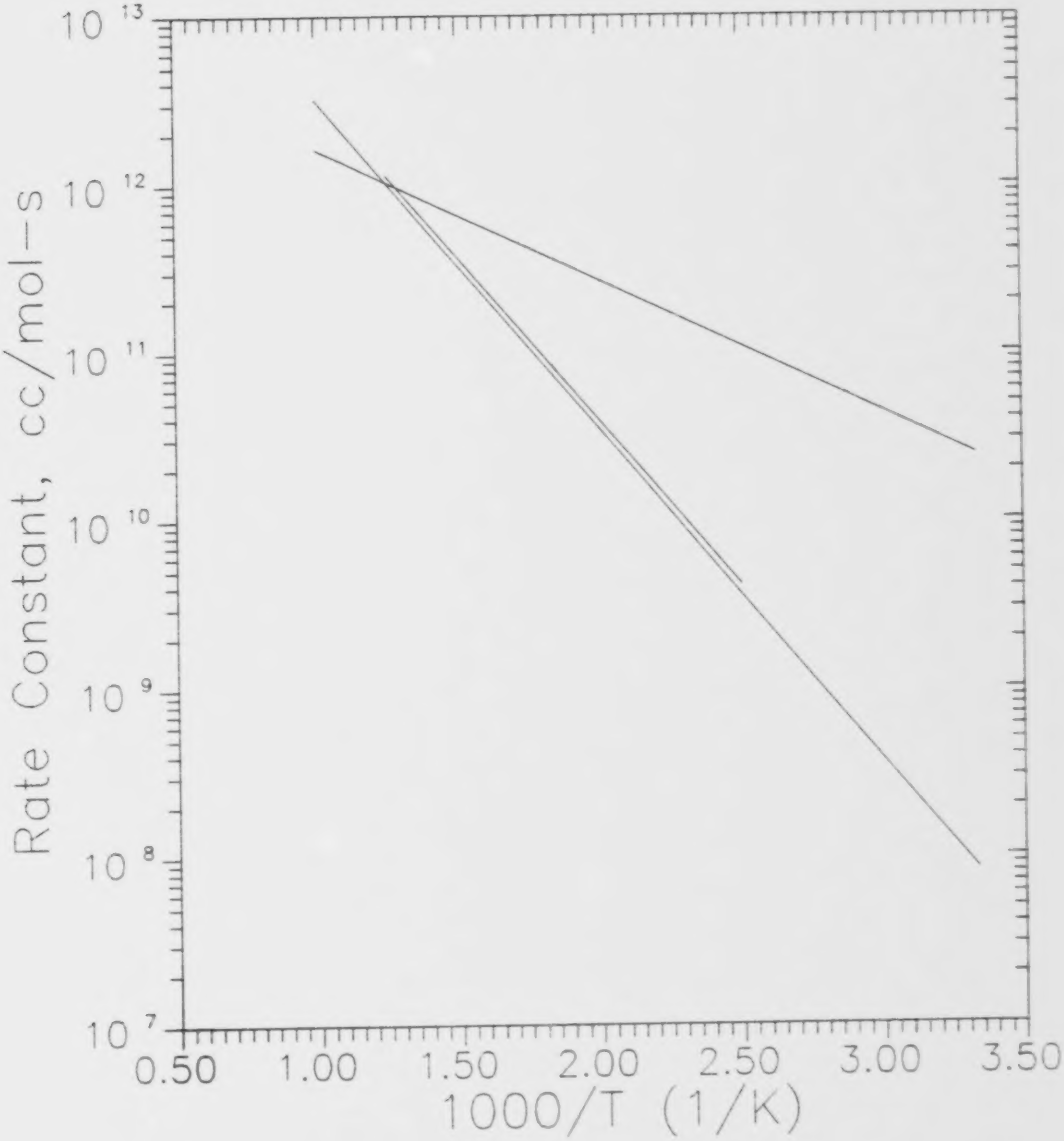

Rate Constant, cc/mol-s
10 12
10 11
10 10
10 9
10 8
10 7
10 6
10 5
10 4
10 3
10 2
0.00
0.40
0.80
1.20
1.60
1000/T (1/K)

**H2O2 + M = HO + HO + M**

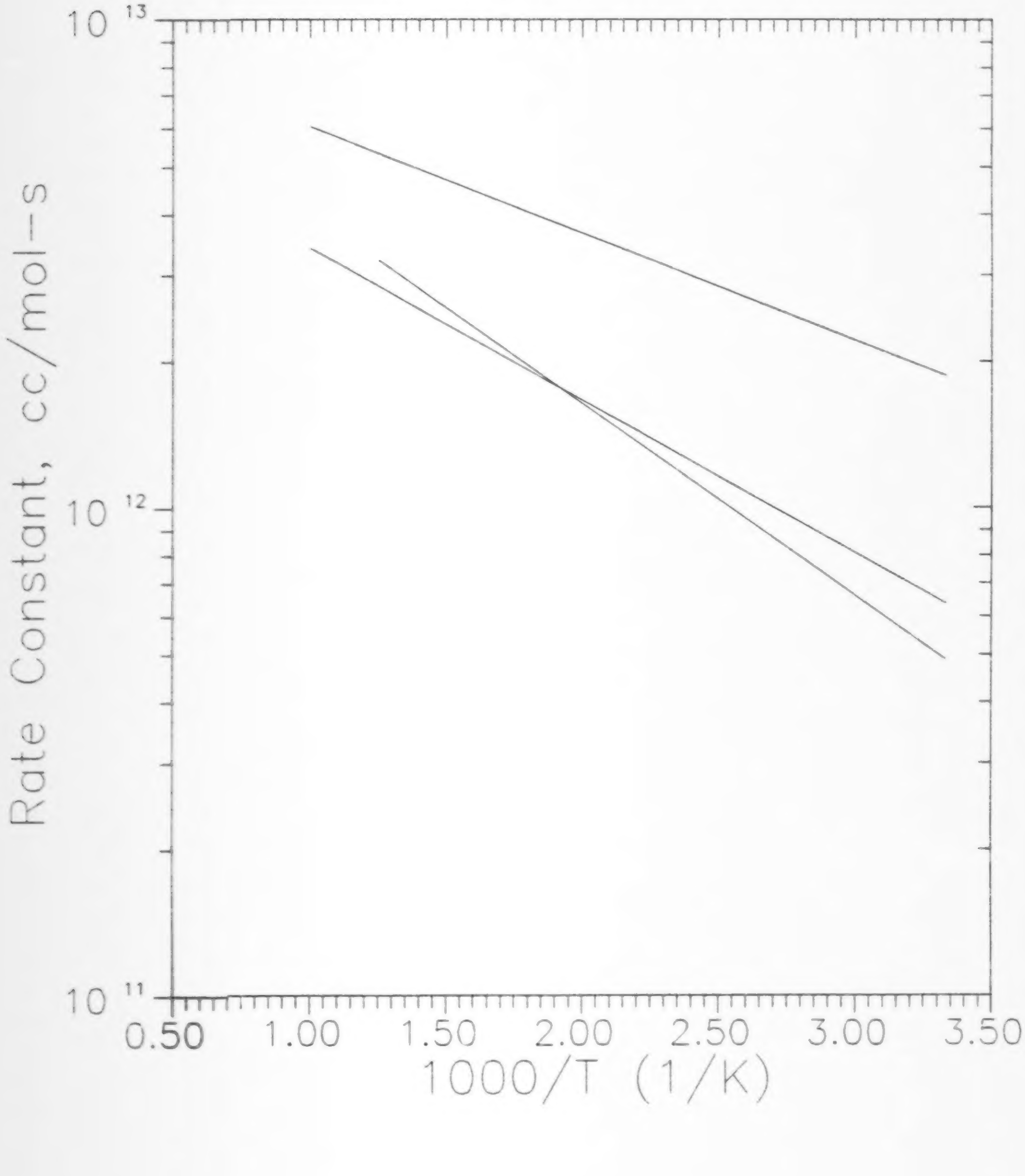


Rate Constant, cc/mol-s
$10^{13}$
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

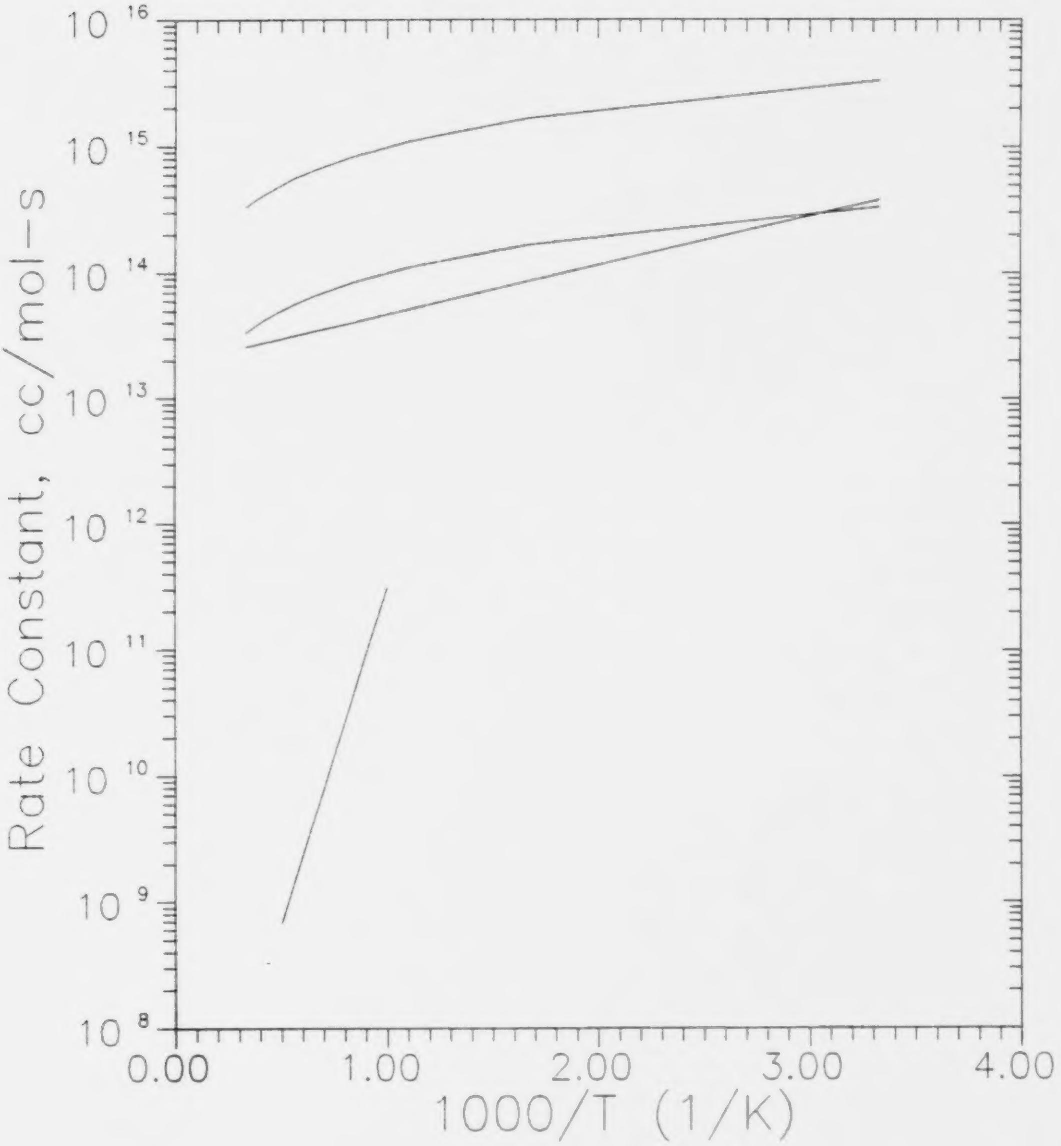
**$H_2O_2$ + H = $HO_2$ + $H_2$**


Rate Constant, cc/mol-s
10 13
10 12
10 11
10 10
10 9
10 8
10 7
0.50
1.00
1.50
2.00
2.50
3.00
3.50
1000/T (1/K)

**H2O2 + H = H2O + HO**



**H2O2 + HO = H2O + HO2**


Rate Constant, cc/mol-s
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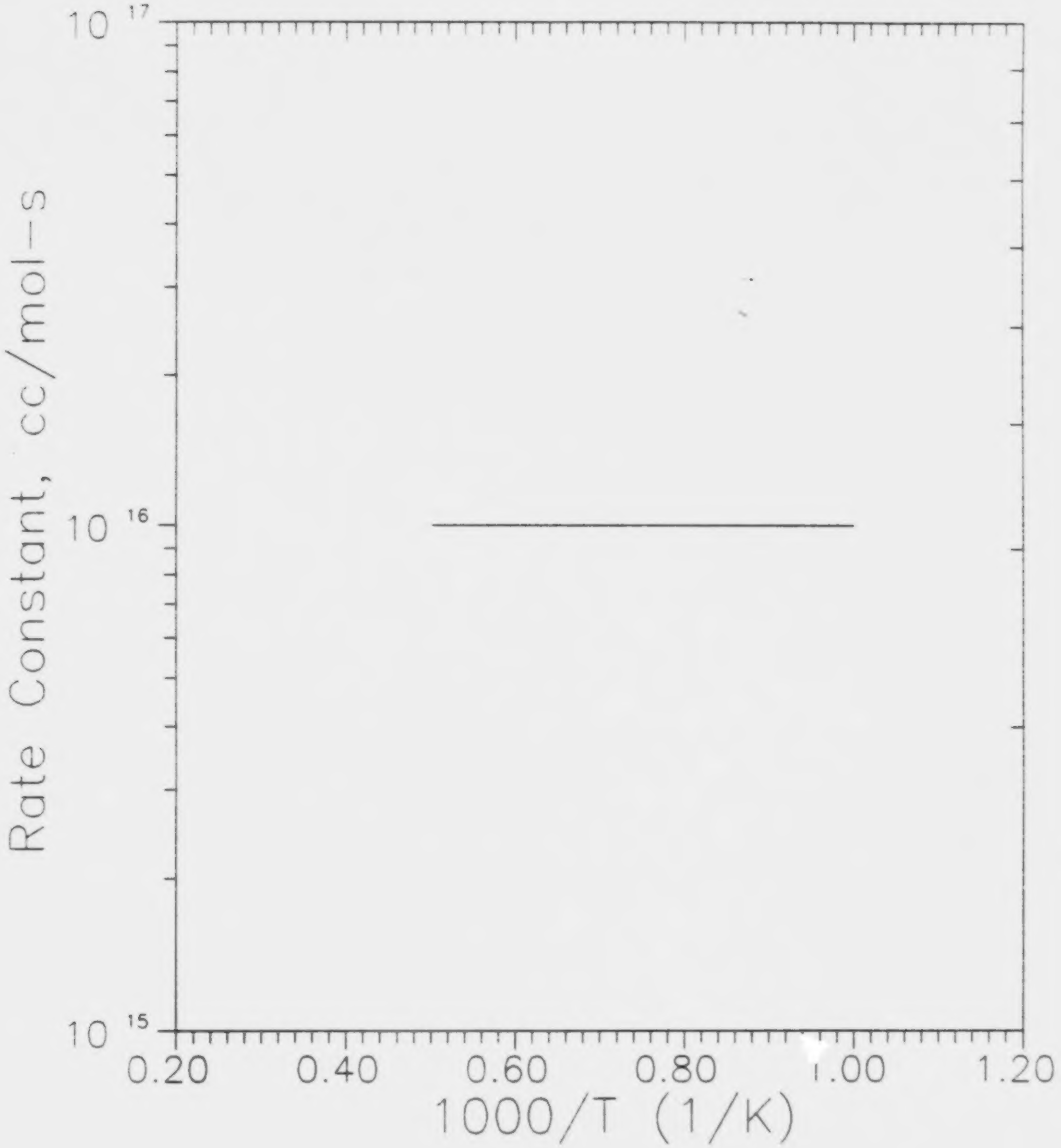
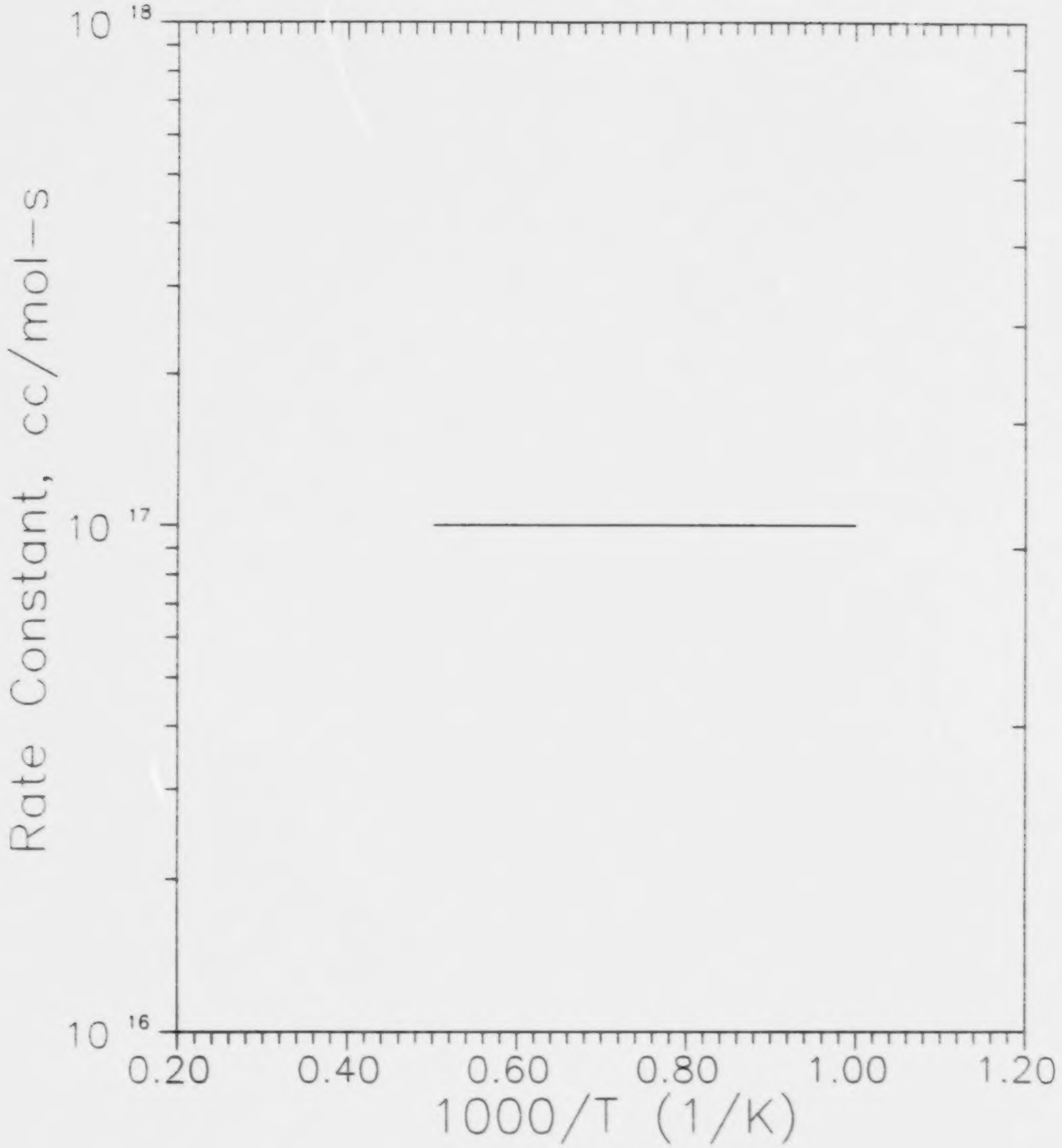
10 14
10 13
10 12
10 11
10 10
10 9
10 8
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**O + O + M = O2 + M**



10 17
10 16
10 15
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**O +H +M =HO +M**


Rate Constant, cc/mol-s
$10^{18}$
$10^{17}$
$10^{16}$
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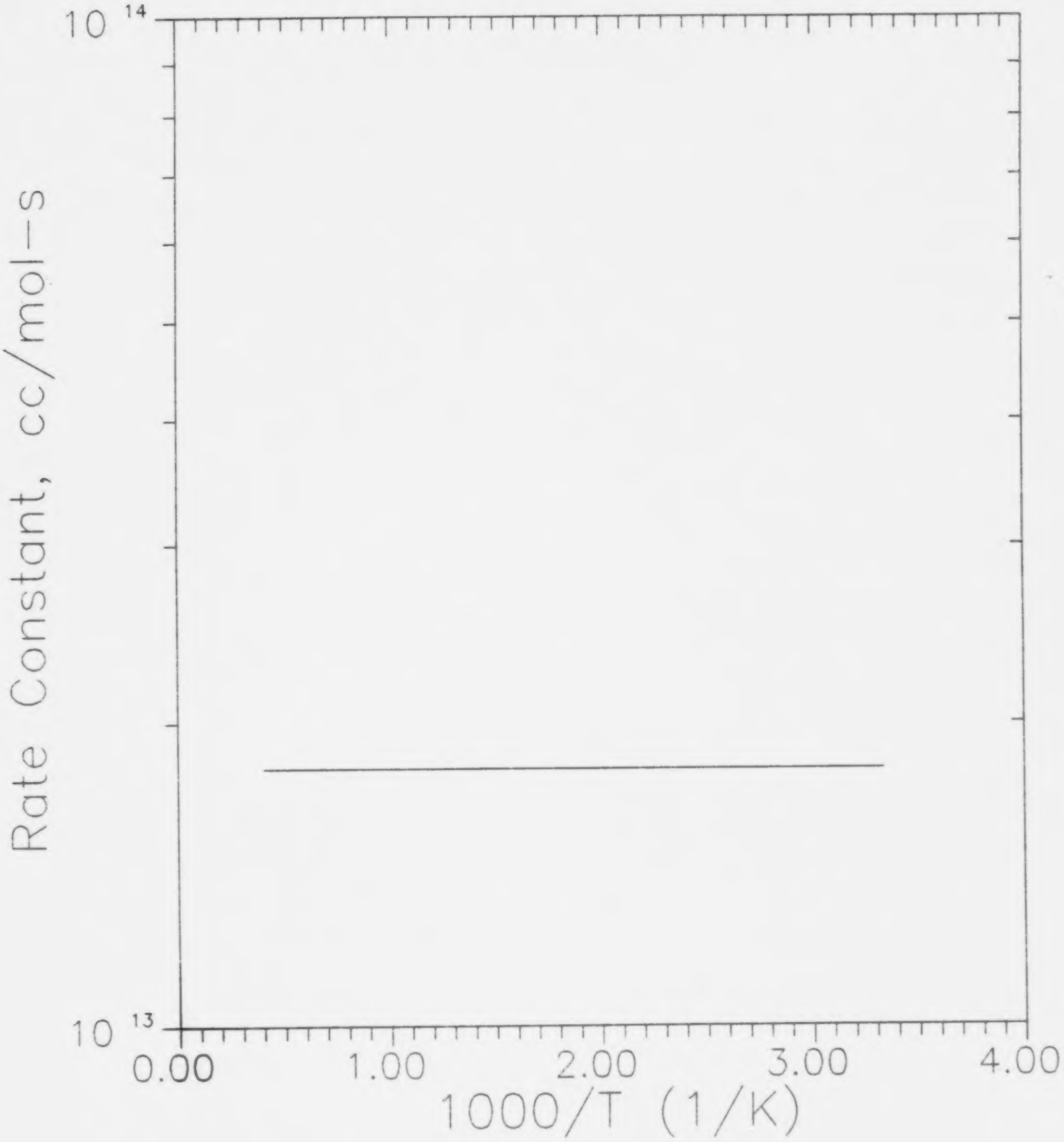
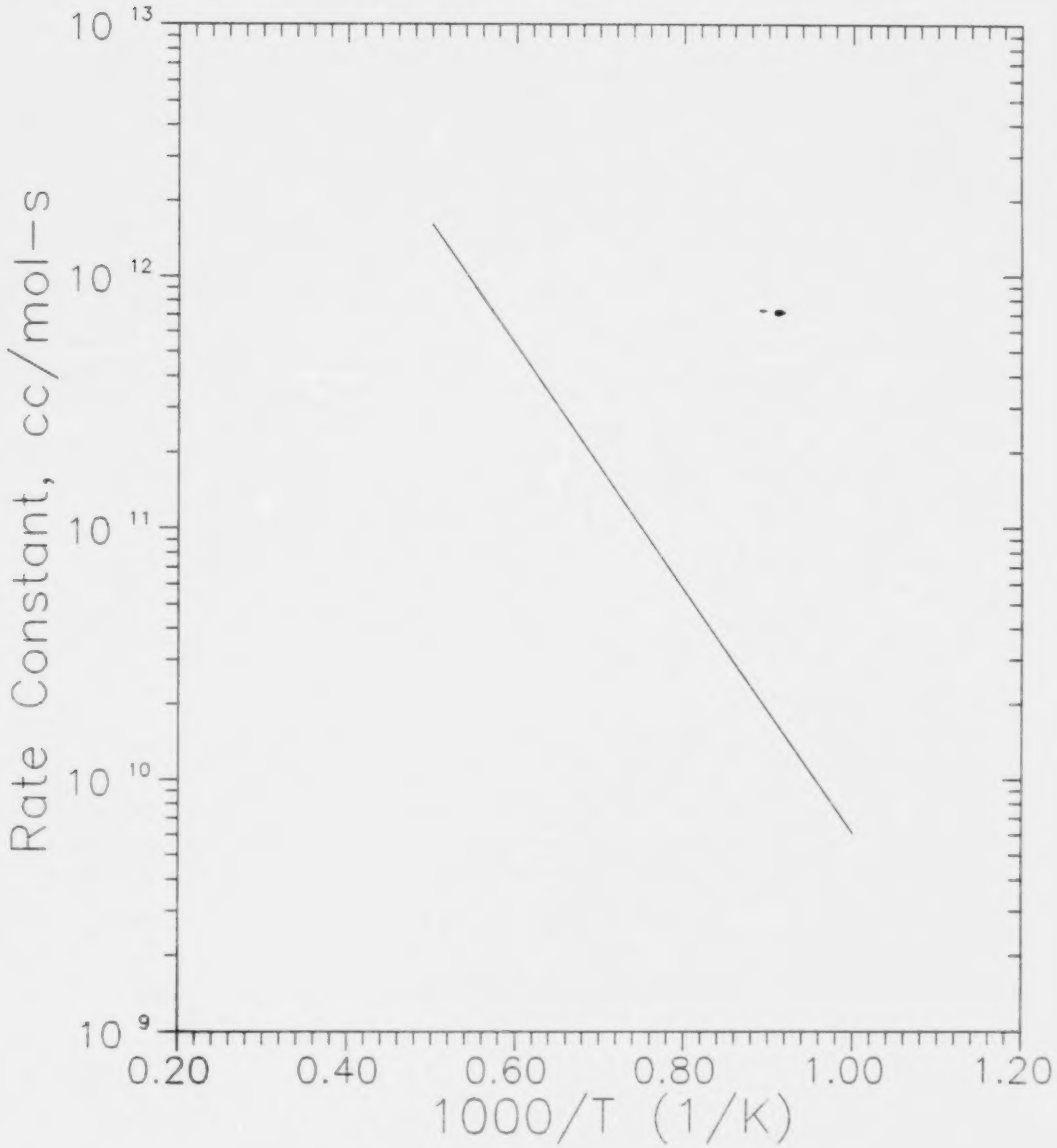
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

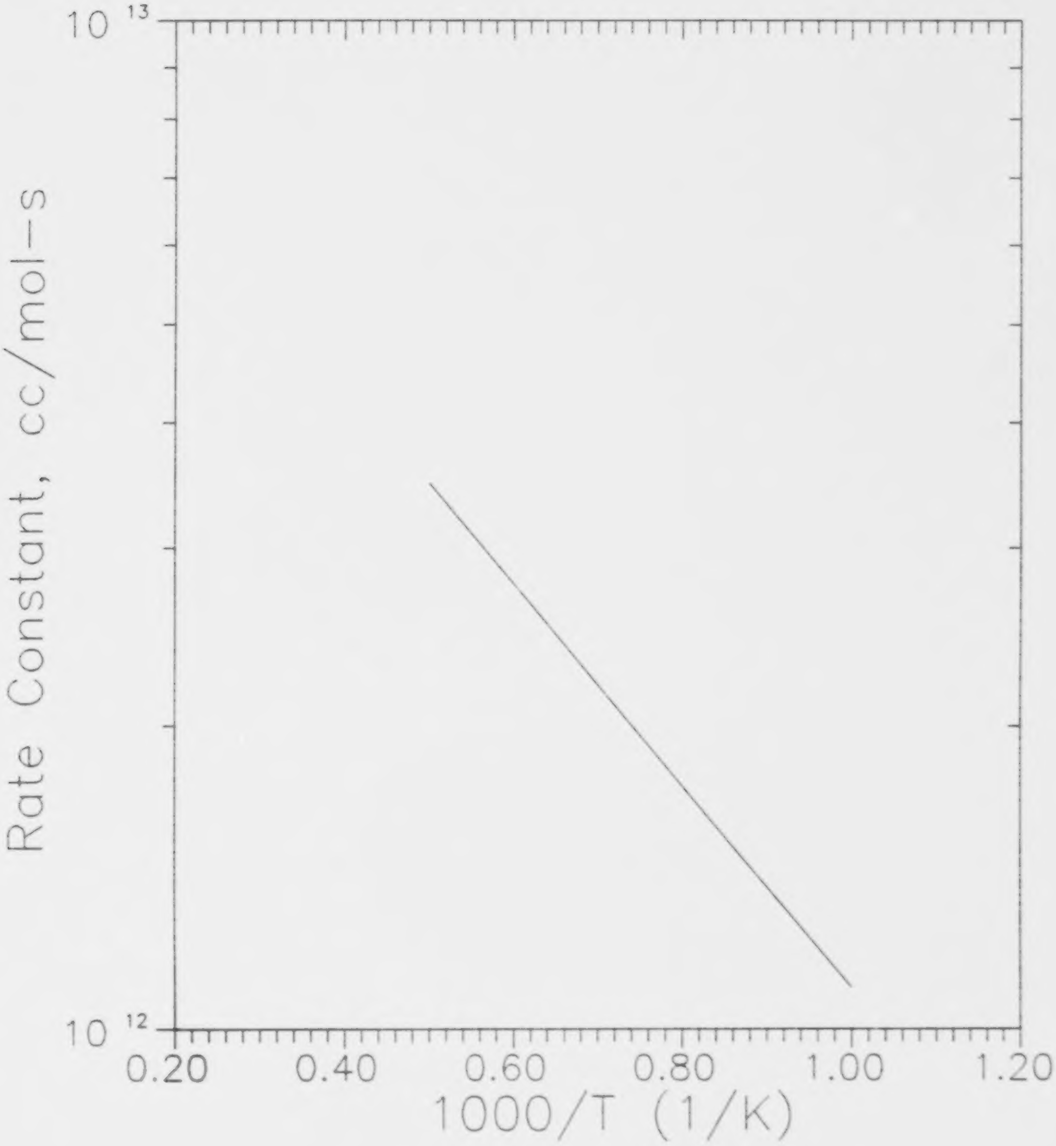
**O + HO + M = HO2 + M**



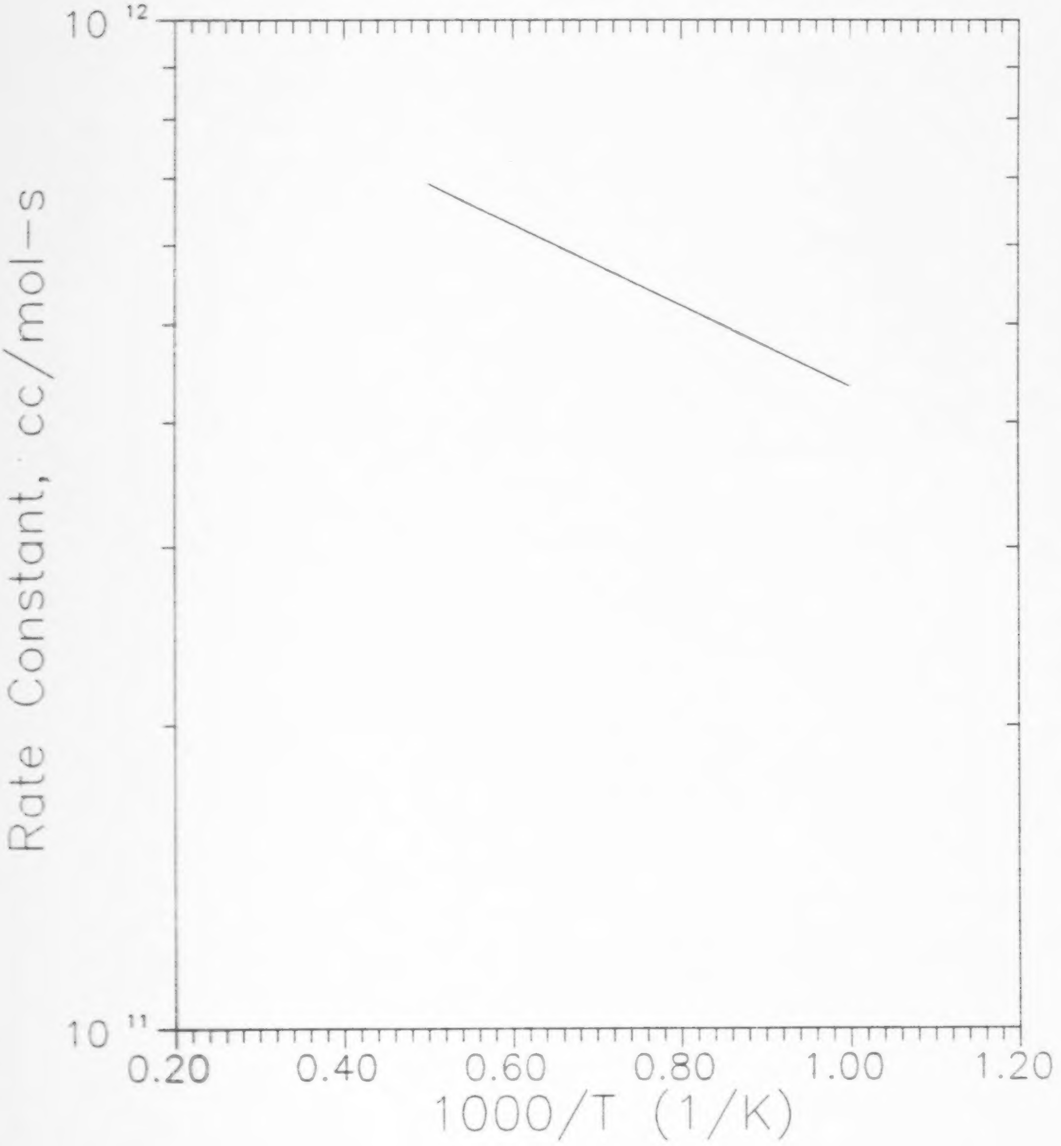
**O + HO = HO2**


10 13
10 12
10 11
10 10
10 9
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**O3 + M = O2 + O + M**

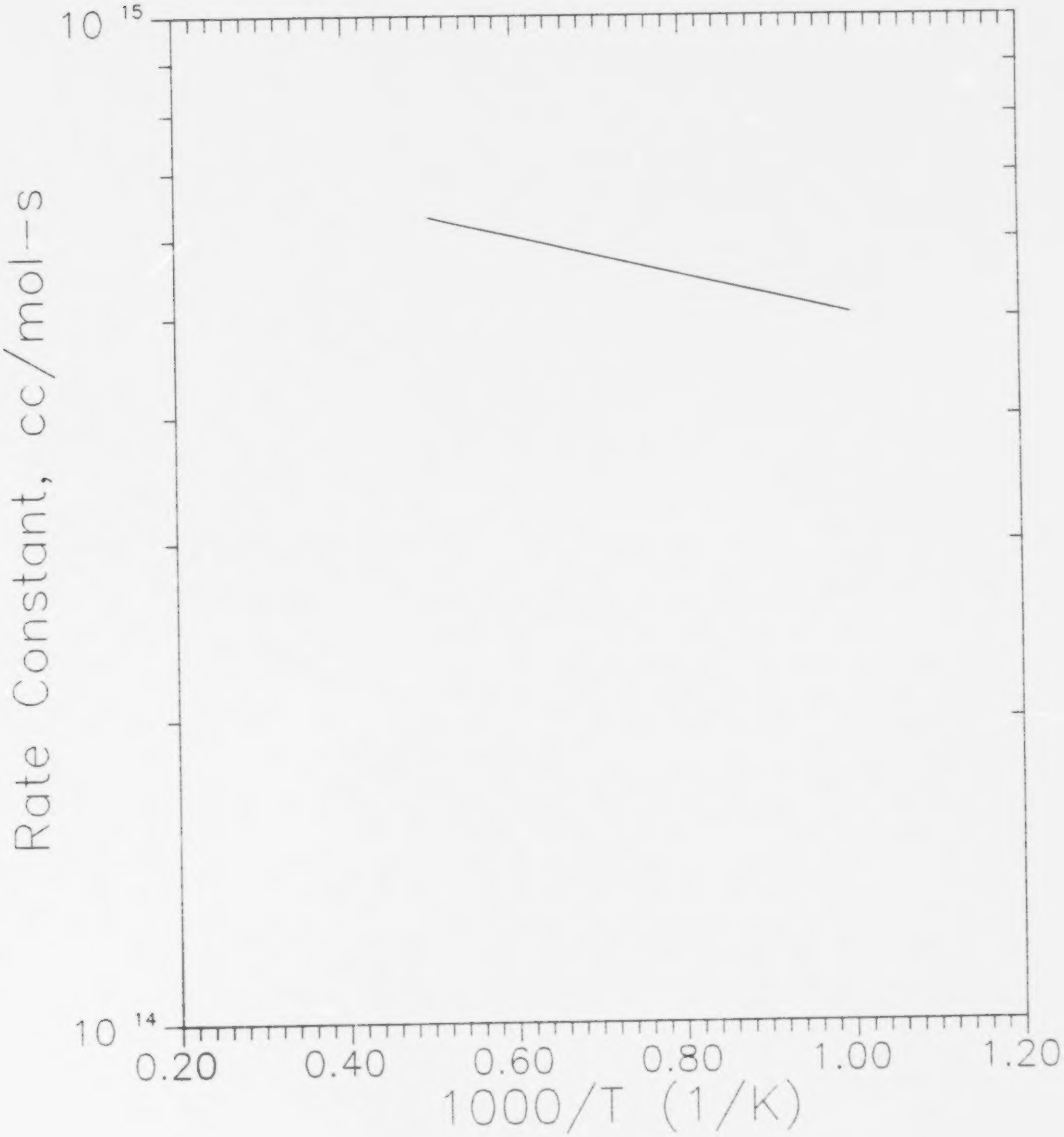

10 $^{13}$
10 $^{12}$
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**O3 + O = O2 + O2**



10 12
10 11
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**O3 + HO = HO2 + O2**


10^15
10^14
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

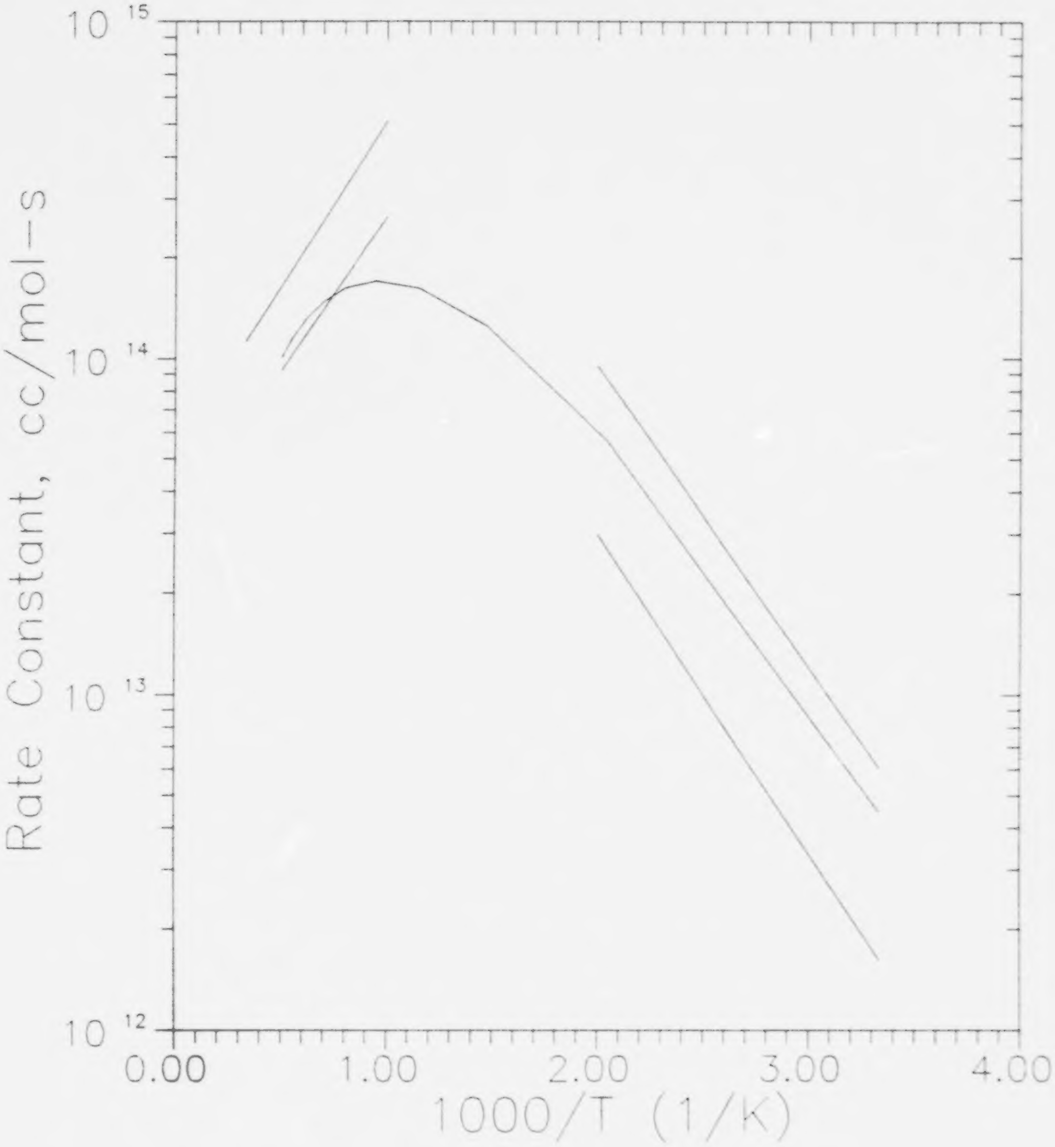
**O3 + H = O2 + HO**

```
*-----------------------------------------------------------------------------*
! File: COMECH.DAT                                                             !
! Saved: 08-04-88 at 11:05:07 am                                     Page  1 !
*-----------------------------------------------------------------------------*

 1CO    + 1O     + 1M     = 1CO2   + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                    3.2E+13 0.000 -4.200  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                      5.9E+15 0.000  4.100   300.0   500.0
Seeker, et al. 1985                      3.8E+24-3.000  6.170   300.0  2000.0
Warnatz, Comb Chem                       5.3E+13 0.000 -4.500  1000.0  3000.0
Tsang and Hampson. 1986                  2.36E15 0.000  4.340   250.0   500.0

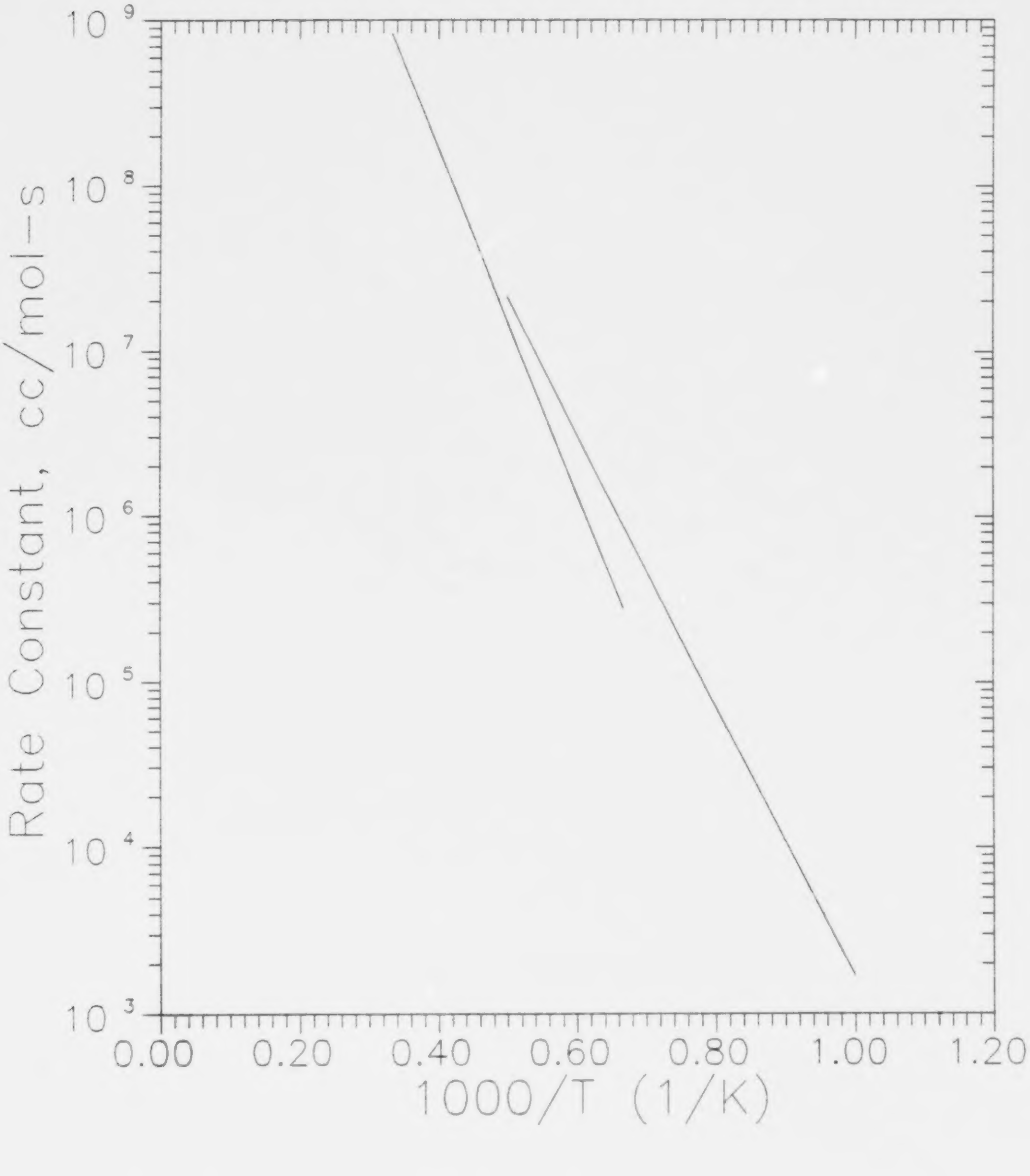
 1CO    + 1O2             = 1CO2   + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                    2.5E+12 0.000 47.700  1500.0  3000.0
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, Comb Chem
Seeker, et al. 1985                      6.9E+07 1.000 34.810  1000.0  2000.0

 1C     + 1O2             = 1CO    + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                    5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986                    2.0E+13 0.000  0.000  1000.0  2000.0
```



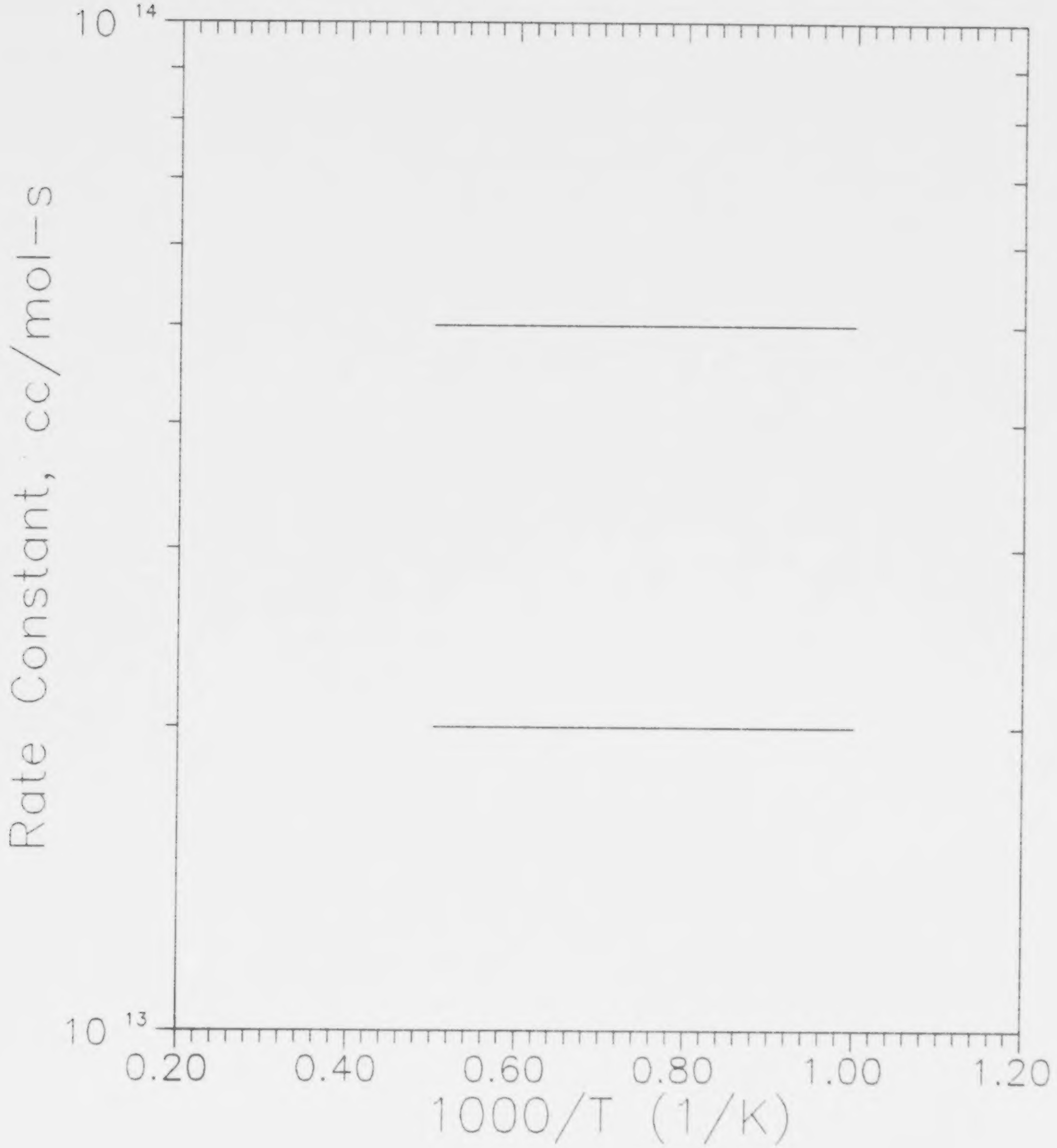
Rate Constant, cc/mol-s
$10^{15}$
$10^{14}$
$10^{13}$
$10^{12}$
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

CO + O + M = CO2 + M



Rate Constant, cc/mol-s
10 9
10 8
10 7
10 6
10 5
10 4
10 3
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CO + O2 = CO2 + O**



Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**C + O2 = CO + O**

```
*---------------------------------------------------------------------------*
!  File: CHMECH.DAT                                                          !
! Saved: 08-04-88 at 11:04:19 am                                     Page  1 !
*---------------------------------------------------------------------------*

 1CH4  + 1M           = 1CH3  + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                 1.0E+17 0.000 88.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                   1.3E+17 0.000 88.400  1875.0  2240.0
Westbrook and Dryer                   2.0E+17 0.000 88.000  1500.0  3000.0
Warnatz, Comb. Chem.

 1CH4  + 1H           = 1CH3  + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                 2.2E+04 3.000  8.750   300.0  1800.0
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, Comb. Chem.
Seeker, et al. 1985                   1.4E+07 2.000  8.840   300.0  1800.0

 1CH4  + 1CH3         = 1C2H5 + 1H2
Forward Rate Parameters:
Seeker, et al. 1985                   1.0E+13 0.000 23.000  1000.0  2000.0

 1CH4  + 1CH3         = 1C2H6 + 1H
Forward Rate Parameters:
Seeker, et al. 1985                   8.0E+13 0.000 40.000  1000.0  2000.0

 1CH4  + 1CH2         = 1CH3  + 1CH3
Forward Rate Parameters:
Glarborg, et al. 1985                 6.0E+14 0.000 14.000  1000.0  2000.0
Glarborg, et al. 1986                 1.3E+13 0.000  9.500  1000.0  2000.0
Seeker, et al. 1985                   1.3E+10 0.700 20.000  1000.0  2000.0

 1CH4  + 1CH          = 1C2H4 + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                 6.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                   1.5E+12 0.000  0.000  1000.0  2000.0

 1CH4  + 1CH          = 1CH3  + 1CH2
Forward Rate Parameters:
Seeker, et al. 1985                   2.5E+11 0.700  6.000  1000.0  2000.0

 1CH4  + 1C           = 1CH   + 1CH3
Forward Rate Parameters:
Glarborg, et al. 1985                 5.0E+13 0.000 24.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH3  + 1CH3         = 1C2H6
Forward Rate Parameters:
Glarborg, et al. 1985                 1.6E+13 0.000 -0.306  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                   1.0E+13 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985                   2.4E+13 0.000  0.000  2500.0  3000.0
Warnatz, Comb. Chem.                  2.4E+14-0.400  0.000   300.0  2000.0

 1CH3  + 1CH3  + 1M   = 1C2H6 + 1M    +
Forward Rate Parameters:
```

```
*----------------------------------------------------------------------------*
!  File: CHMECH.DAT                                                          !
! Saved: 08-04-88 at 11:04:19 am                                    Page  2  !
*----------------------------------------------------------------------------*

This work                                  1.87E32-4.740  0.000  1000.0  2500.0

 1CH3  + 1CH3        = 1C2H5 + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                      8.0E+14 0.000 26.630  1500.0  3000.0
Warnatz, Comb. Chem.
Westbrook and Dryer                        7.9E+14 0.000 26.520  1000.0  2000.0
Reverse Rate Parameters:
Seeker, et al. 1985                        3.7E+13 0.000  0.000   500.0   750.0
Warnatz, Comb. Chem.                       3.0E+13 0.000  0.000   300.0  1500.0
Glarborg, et al. 1986                      4.0E+13 0.000  0.000   300.0  1000.0

 1CH3  + 1CH3        = 1C2H4 + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                      2.1E+14 0.000 19.200  1500.0  2500.0
Glarborg, et al. 1986
Westbrook and Dryer                        1.0E+16 0.000 32.000  1500.0  2500.0
Warnatz, Comb. Chem.

 1CH3  + 1M          = 1CH2  + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                      1.9E+16 0.000 91.600  2150.0  2850.0
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, Comb. Chem.                       1.0E+16 0.000 90.600  1500.0  3000.0

 1CH3  + 1H          = 1CH2  + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                      9.0E+13 0.000 15.100  1000.0  2000.0
Glarborg, et al. 1986
Reverse Rate Parameters:
Seeker, et al. 1985                        1.0E+11 0.500  5.730  1000.0  2000.0

 1CH3  + 1CH2        = 1C2H4 + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                      3.0E+13 0.000  0.000   300.0  1000.0
Glarborg, et al. 1986
Seeker, et al. 1985                        6.0E+13 0.000  0.000   300.0   301.0
Warnatz, Comb. Chem.                       4.0E+13 0.000  0.000   300.0  2500.0

 1CH3  + 1C2H4       = 1C2H3 + 1CH4
Forward Rate Parameters:
Seeker, et al. 1985                        5.0E+12 0.000 13.000   300.0  1000.0
Warnatz, Comb. Chem.                       4.2E+11 0.000 10.760   300.0  1000.0

 1CH3  + 1C2H5       = 1C2H4 + 1CH4
Forward Rate Parameters:
Seeker, et al. 1985                        2.5E+11 0.000  0.000  1000.0  2000.0

 1CH3  + 1C2H6       = 1C2H5 + 1CH4
Forward Rate Parameters:
Glarborg, et al. 1985                      5.5E-01 4.000  8.280   300.0  1800.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985
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Warnatz, Comb. Chem.

 1CH3  + 1CH           = 1C2H3 + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                  3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH3  + 1C            = 1C2H2 + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                  5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH2  + 1C2H6         = 1C2H5 + 1CH3
Forward Rate Parameters:
Seeker, et al. 1985                    1.2E+13 0.000 15.700  1000.0  2000.0
Glarborg, et al. 1986                  2.2E+13 0.000  8.660  1000.0  2000.0

 1CH2  + 1C2H3         = 1C2H2 + 1CH3
Forward Rate Parameters:
Glarborg, et al. 1985                  3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer

 1CH2  + 1H            = 1CH   + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                  1.4E+19-2.000  0.000   300.0  2000.0
Glarborg, et al. 1986                  7.3E+17-1.560  0.000   300.0  2800.0
Westbrook and Dryer                    2.5E+11 0.670 25.700  1000.0  3000.0
Warnatz, Comb. Chem.                   4.0E+13 0.000  0.000   300.0  2500.0
This work                              6.19E17-1.450  0.000  1000.0  2500.0
Reverse Rate Parameters:
Seeker, et al. 1985                    1.2E+13 0.000  0.000  1000.0  2000.0

 1CH2  + 1CH           = 1C2H2 + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                  4.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH2  + 1CH2          = 1C2H2 + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                  3.2E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985
Westbrook and Dryer

 1CH2  + 1CH2          = 1C2H3 + 1H
Forward Rate Parameters:
Westbrook and Dryer                    5.0E+12 0.000  0.000  1000.0  2000.0

 1CH2  + 1CH2          = 1CH3  + 1CH
Forward Rate Parameters:
Seeker, et al. 1985                    5.0E+11 0.500  6.000  1000.0  2000.0

 1CH2  + 1C2H2         = 1CH3  + 1C2H
Forward Rate Parameters:
```

```
Seeker, et al. 1985                        1.0E+12 0.000  0.000  1000.0  2000.0


 1CH2  + 1C2H4         = 1CH3  + 1C2H3
Forward Rate Parameters:
Seeker, et al. 1985                        1.1E+13 0.000 12.400  1000.0  2000.0

 1CH2  + 1C            = 1C2H  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                      5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH   + 1C2H2         = 1C2H3 + 1H
Forward Rate Parameters:
Glarborg, et al. 1986                      1.3E+14 0.000  0.000  1000.0  2000.0

 1CH   + 1C2H2         = 1CH2  + 1C2H
Forward Rate Parameters:
Seeker, et al. 1985                        7.1E+13 0.000 11.920  1000.0  2000.0

 1CH   + 1H            = 1C    + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                      5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1C2H6 + 1H            = 1C2H5 + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                      5.4E+02 3.500  5.200   300.0  1800.0
Glarborg, et al. 1986
Seeker, et al. 1985
Westbrook and Dryer
Warnatz, Comb. Chem.

 1C2H5 + 1C2H3         = 1C2H4 + 1C2H4
Forward Rate Parameters:
Seeker, et al. 1985                        3.2E+17 0.000 35.600  1000.0  2000.0

 1C2H5 + 1C2H5         = 1C2H4 + 1C2H6
Forward Rate Parameters:
Seeker, et al. 1985                        5.0E+10 0.000  0.000   300.0   400.0
Warnatz, Comb. Chem.                       1.4E+12 0.000  0.000   300.0  1200.0

 1C2H5 + 1H            = 1C2H4 + 1H2
Forward Rate Parameters:
Seeker, et al. 1985                        1.9E+12 0.000  0.000  1000.0  2000.0

 1C2H5 + 1M            = 1C2H4 + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                      1.0E+17 0.000 31.000   700.0  1500.0
Glarborg, et al. 1986
Warnatz, Comb. Chem.
Westbrook and Dryer                        2.0E+15 0.000 30.000   700.0  1500.0
This work                                  4.11E39-7.050 39.700  1000.0  2500.0

 1C2H4 + 1H            = 1C2H5
```

```
Forward Rate Parameters:
Seeker, et al. 1985                       1.0E+13 0.000  1.500   300.0  2000.0
Warnatz, Comb. Chem.

 1C2H4 + 1M            = 1C2H2 + 1H2    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                     2.6E+17 0.000 79.350  1500.0  2500.0
Warnatz, Comb. Chem.
Glarborg, et al. 1986                     2.6E+17 0.000 79.290  1500.0  2500.0
Seeker, et al. 1985
Westbrook and Dryer                       9.3E+16 0.000 77.200  1500.0  2500.0

 1C2H4 + 1M            = 1C2H3 + 1H     + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                     2.6E+17 0.000 96.600  1700.0  2200.0
Glarborg, et al. 1986
Warnatz, Comb. Chem.
Seeker, et al. 1985                       3.8E+17 0.000 98.170  1000.0  2000.0
Westbrook and Dryer                       6.3E+18 0.000108.720  1050.0  1850.0

 1C2H4 + 1H            = 1C2H3 + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                     1.1E+14 0.000  8.500  1200.0  1700.0
Glarborg, et al. 1986
Seeker, et al. 1985
Westbrook and Dryer                       1.5E+07 2.000  6.000  1000.0  2000.0
Warnatz, Comb. Chem.                      1.5E+14 0.000 10.210   700.0  2000.0

 1C2H4 + 1C2H4         = 1C2H3 + 1C2H5
Forward Rate Parameters:
Westbrook and Dryer                       5.0E+14 0.000 64.700  1000.0  2000.0

 1C2H3 + 1M            = 1C2H2 + 1H     + 1M
Forward Rate Parameters:
Glarborg, et al. 1986                     7.9E+14 0.000 31.500  1200.0  1700.0
Westbrook and Dryer
Seeker, et al. 1985
Warnatz, Comb. Chem.                      3.0E+15 0.000 32.000   500.0  2500.0
This work                                 3.06E44-8.250 49.600  1000.0  2500.0
Reverse Rate Parameters:
Glarborg, et al. 1985                     5.5E+12 0.000  2.410  1000.0  2000.0

 1C2H3 + 1H            = 1C2H2 + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                     6.0E+12 0.000  0.000   300.0   301.0
Glarborg, et al. 1986                     4.0E+13 0.000  0.000   300.0   301.0
Westbrook and Dryer                       2.0E+13 0.000  2.500  2000.0  2540.0
Seeker, et al. 1985                       1.0E+13 0.000  0.000  2000.0  2540.0
Warnatz, Comb. Chem.                      2.0E+13 0.000  0.000   300.0  2500.0

 1C2H3 + 1C2H          = 1C2H2 + 1C2H2
Forward Rate Parameters:
Glarborg, et al. 1985                     3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer
```

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*------------------------------------------------------------------------------*
!  File: CHMECH.DAT                                                            !
! Saved: 08-04-88 at 11:04:19 am                                      Page  6 !
*------------------------------------------------------------------------------*

 1C2H2 + 1M            = 1C2H   + 1H     + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                        4.2E+16 0.000107.000  1700.0  3000.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985
Warnatz, Comb. Chem.                         4.0E+16 0.000107.000  1500.0  3000.0

 1C2H2 + 1H            = 1C2H   + 1H2
Forward Rate Parameters:
Westbrook and Dryer                          2.0E+14 0.000 19.000  1000.0  1700.0
Seeker, et al. 1985                          7.8E+00 3.200  0.500  1700.0  3000.0
Warnatz, Comb. Chem.                         6.0E+13 0.000 23.700   300.0  3000.0
Reverse Rate Parameters:
Glarborg, et al. 1985                        4.1E+06 2.390  0.860  1000.0  2000.0
Glarborg, et al. 1986
```
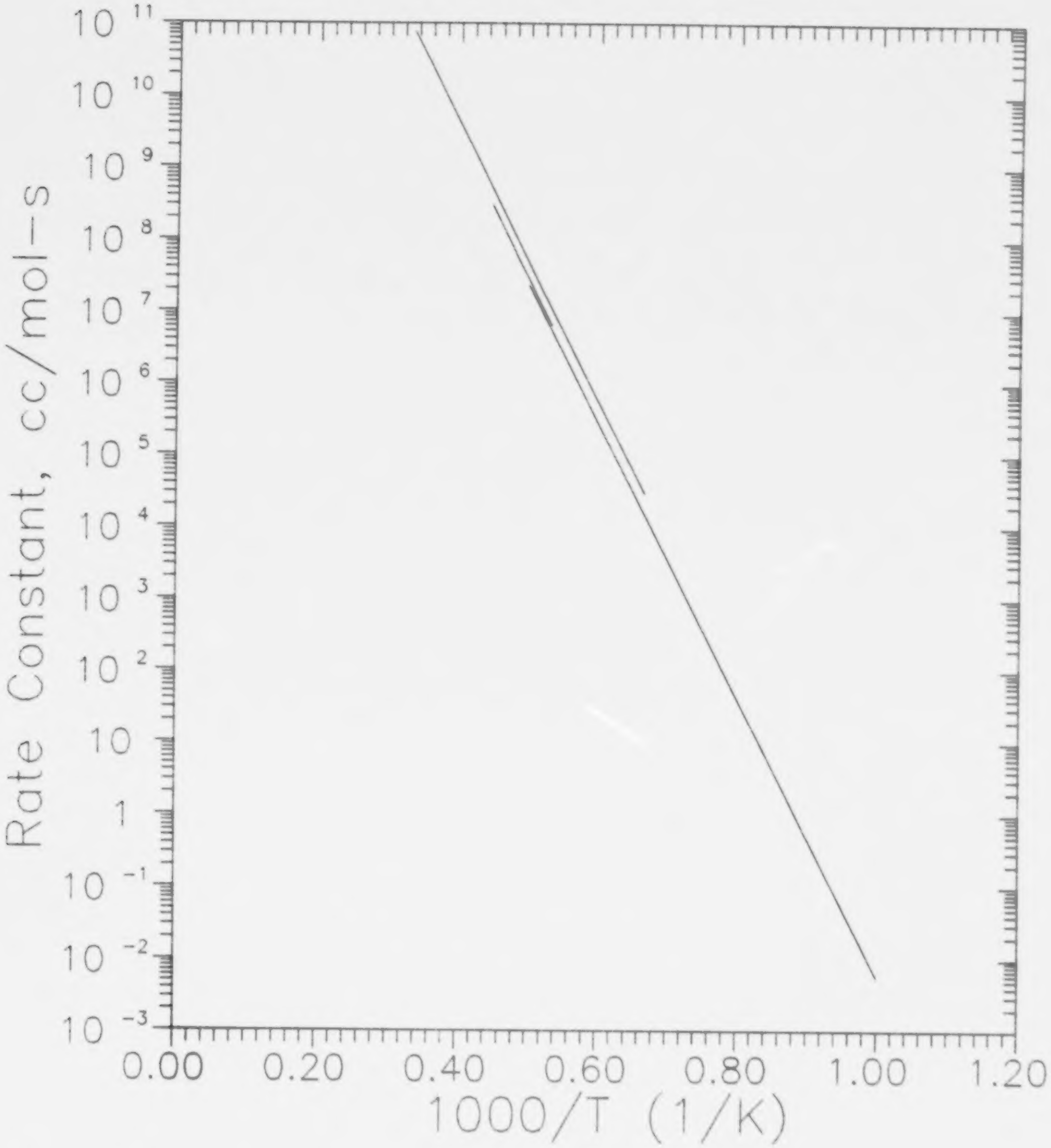
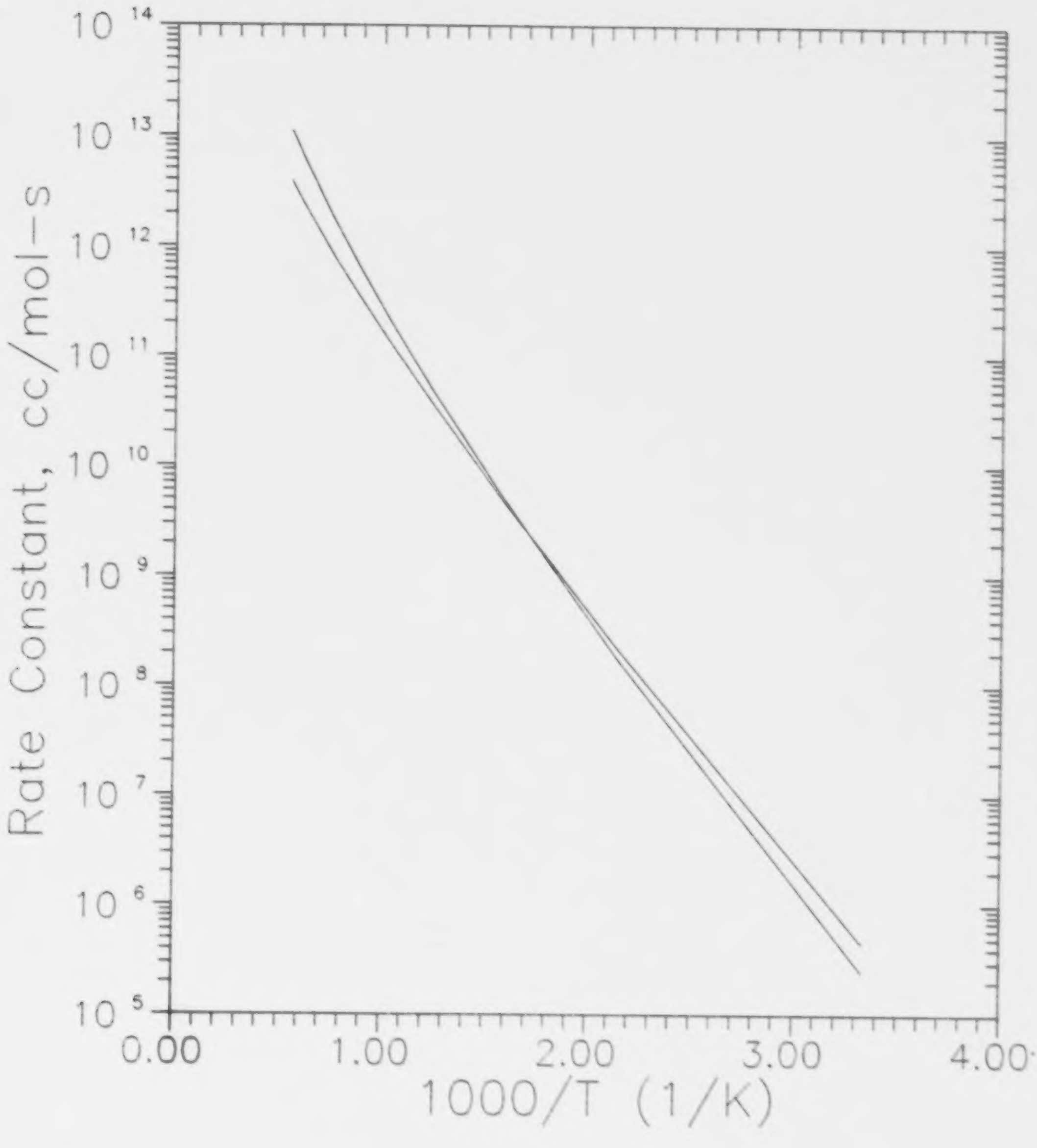
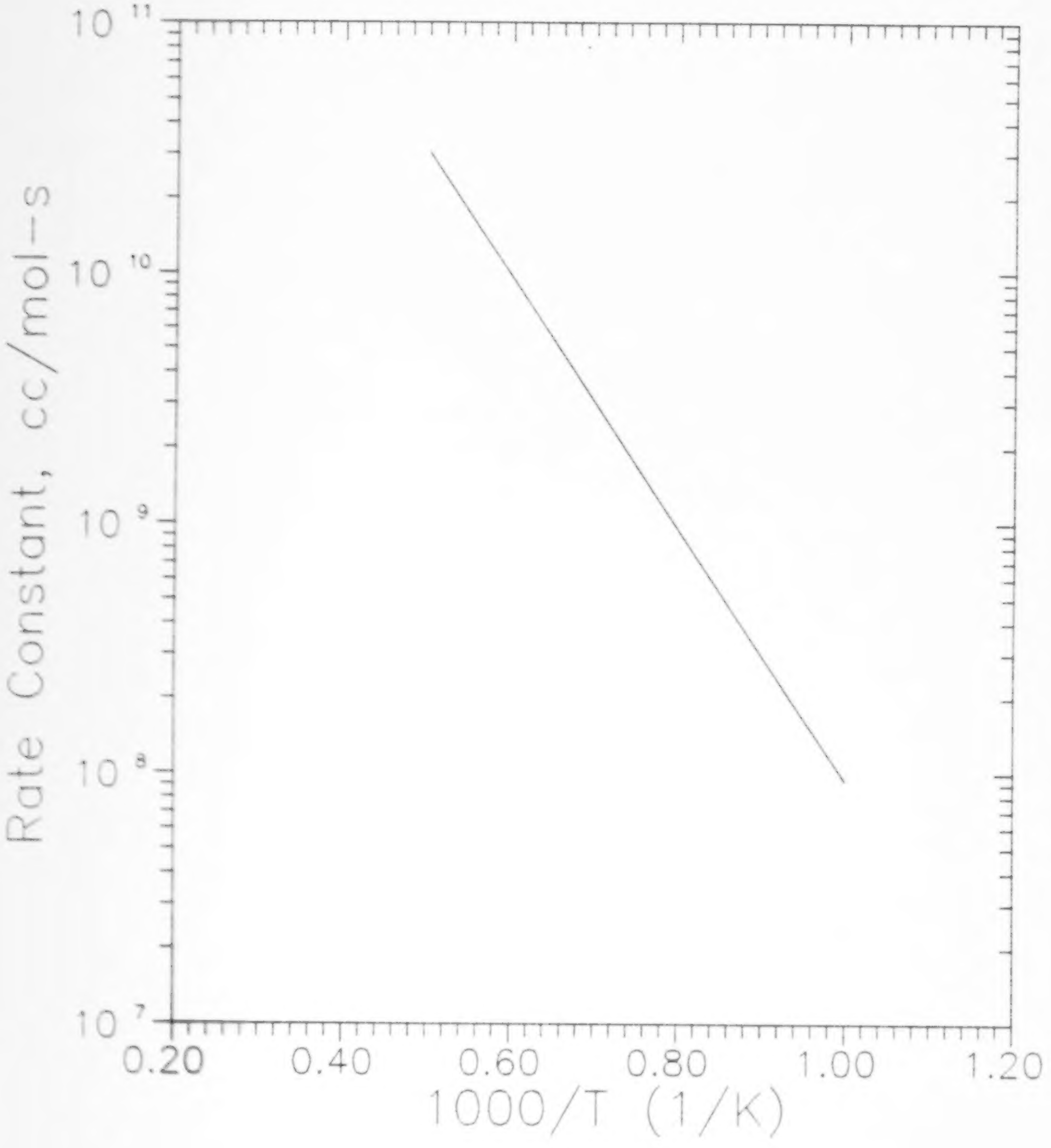



10^11
10^10
10^9
10^8
10^7
10^6
10^5
10^4
10^3
10^2
10
1
10^-1
10^-2
10^-3
Rate Constant, cc/mol-s
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

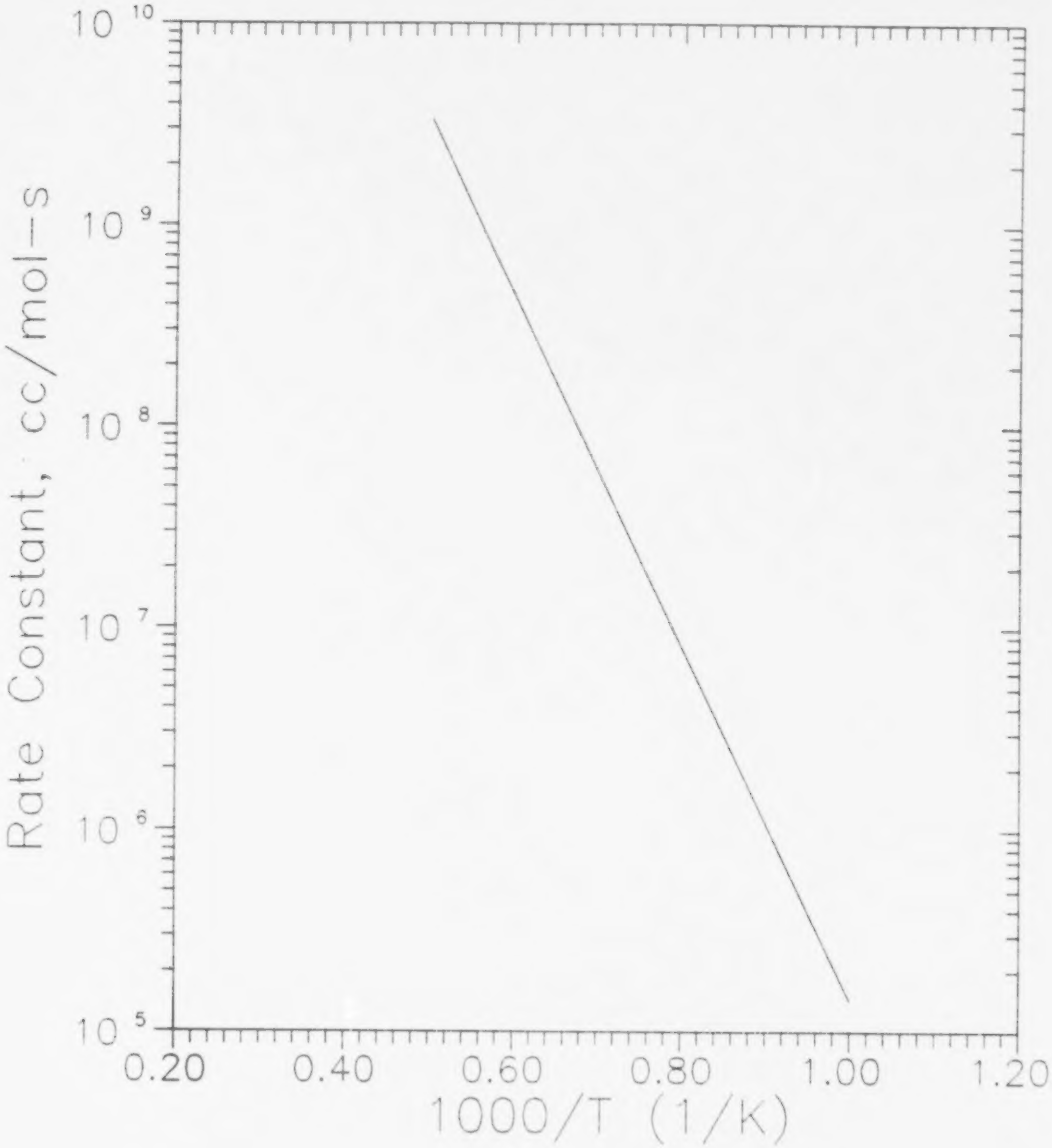
**CH4 + M = CH3 + H + M**


Rate Constant, cc/mol-s
10 14
10 13
10 12
10 11
10 10
10 9
10 8
10 7
10 6
10 5
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

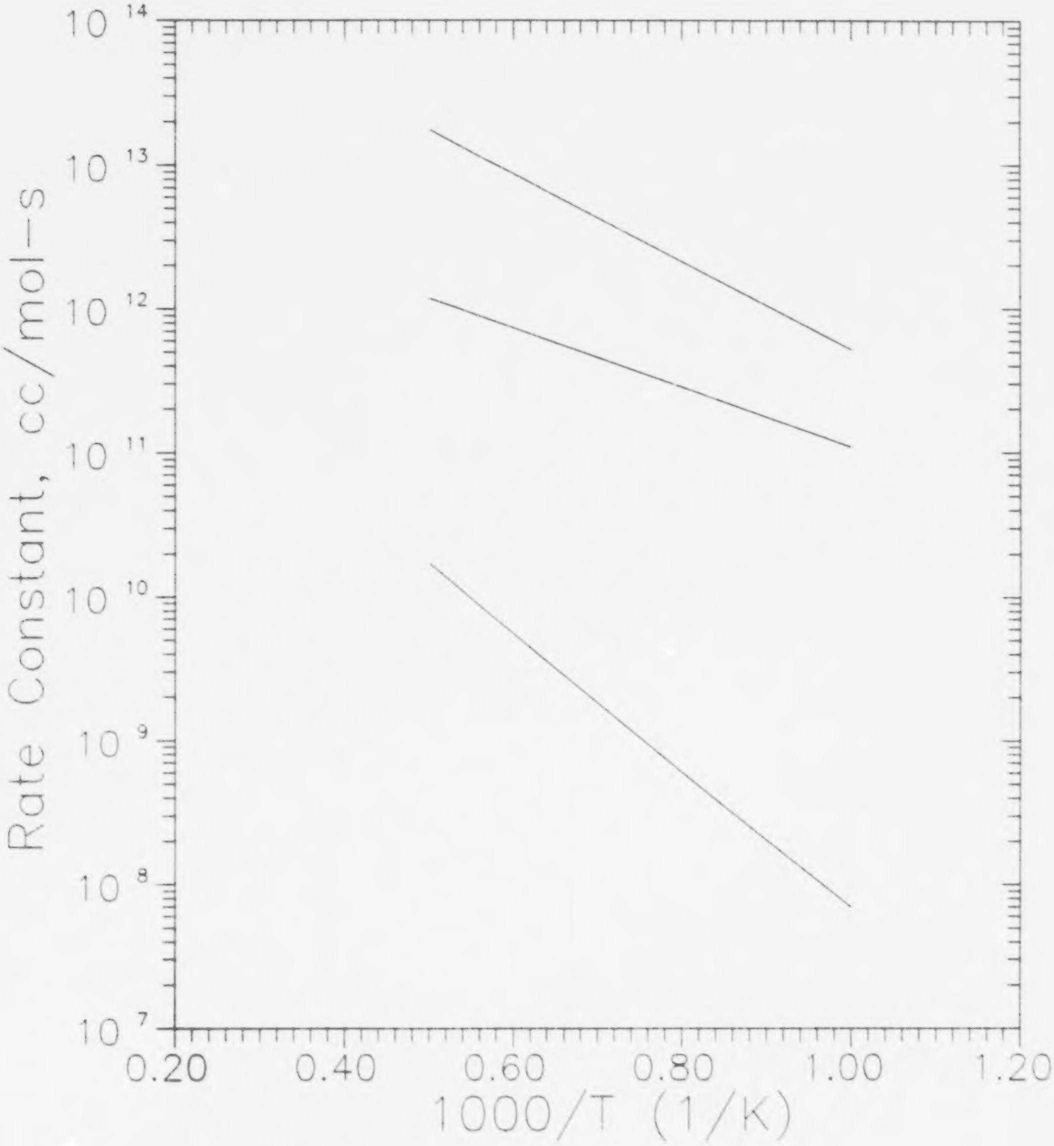
**CH4 + H = CH3 + H2**



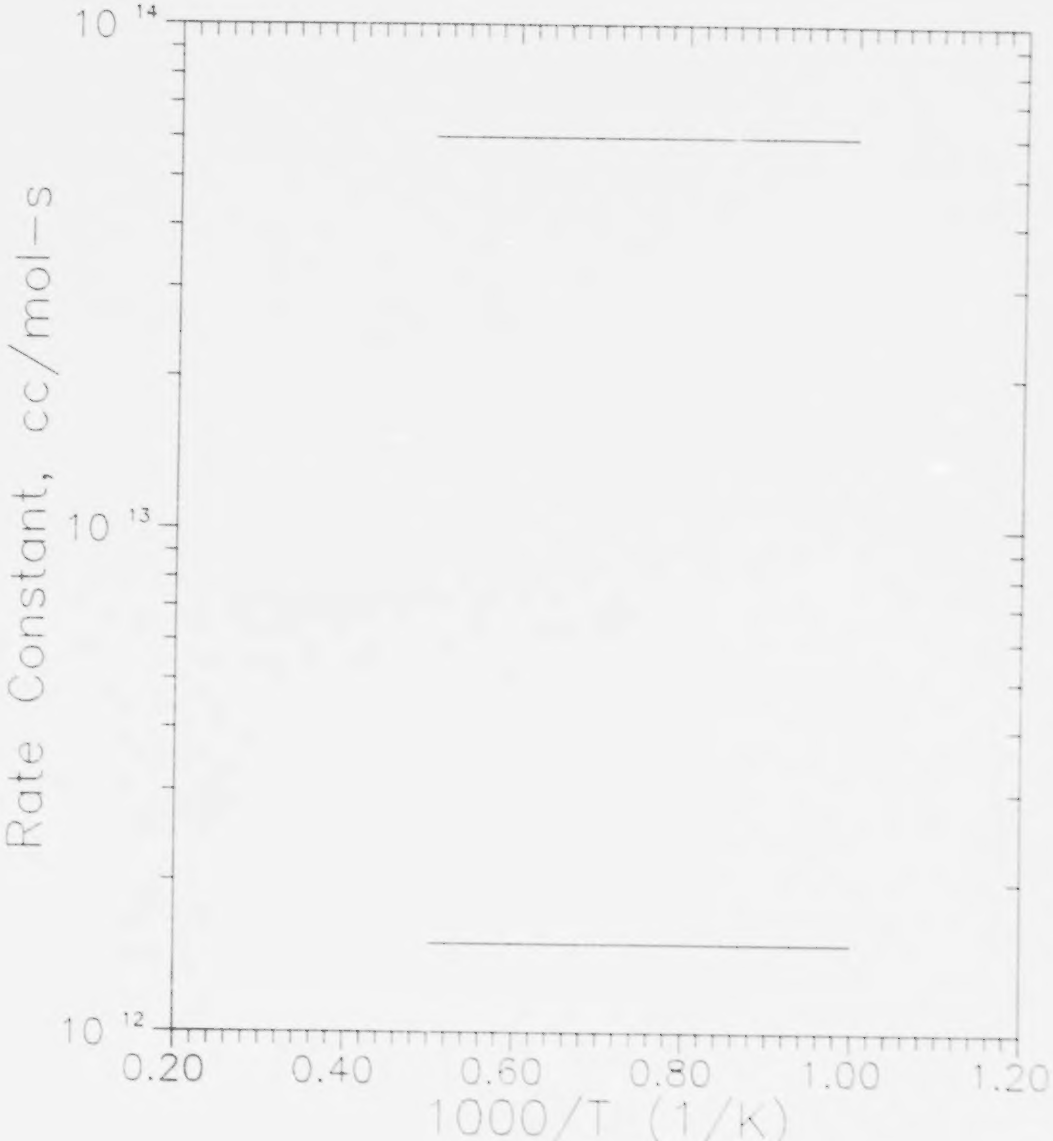
**CH4 + CH3 = C2H5 + H2**



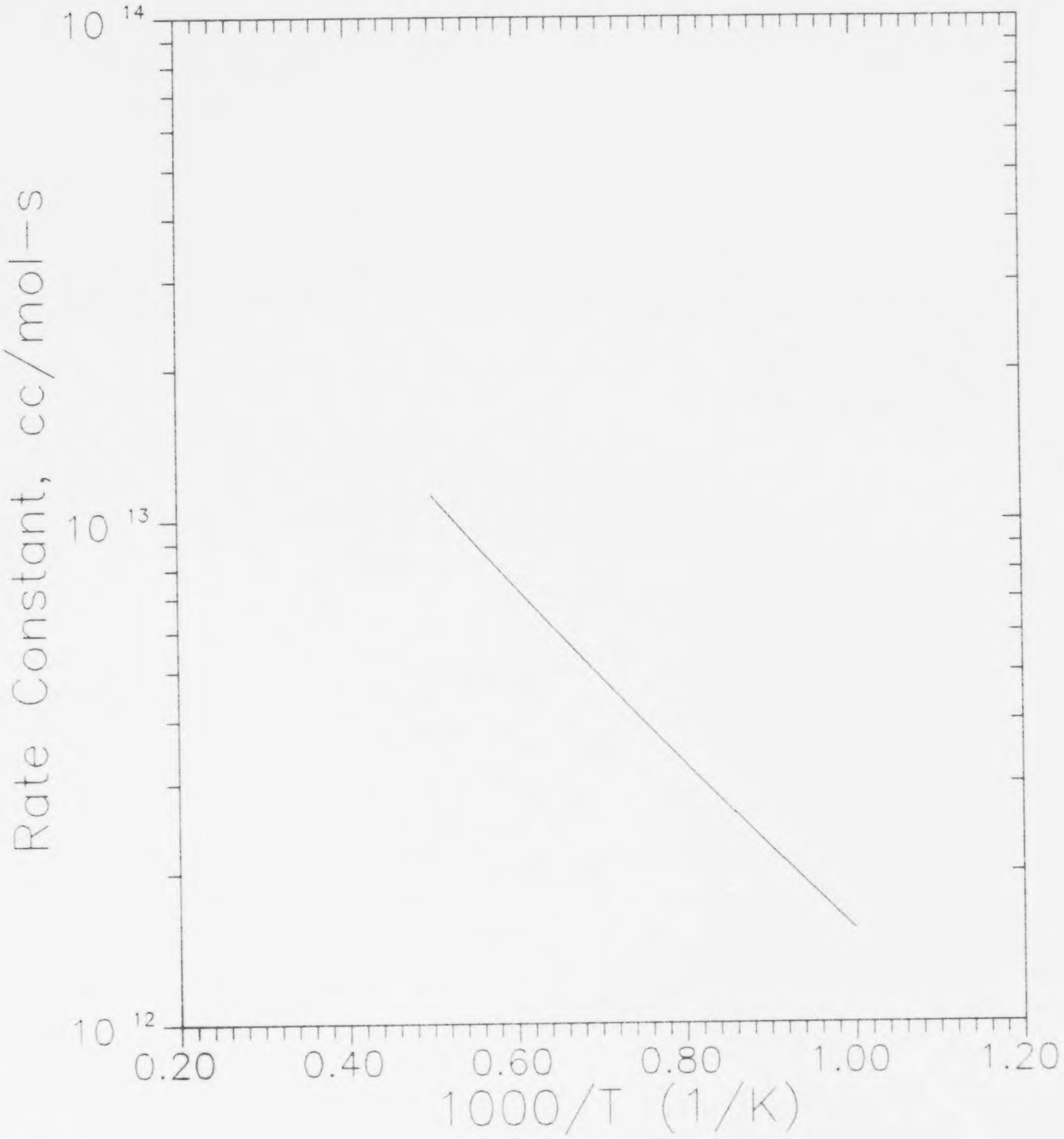
**$CH_4 + CH_3 = C_2H_6 + H$**



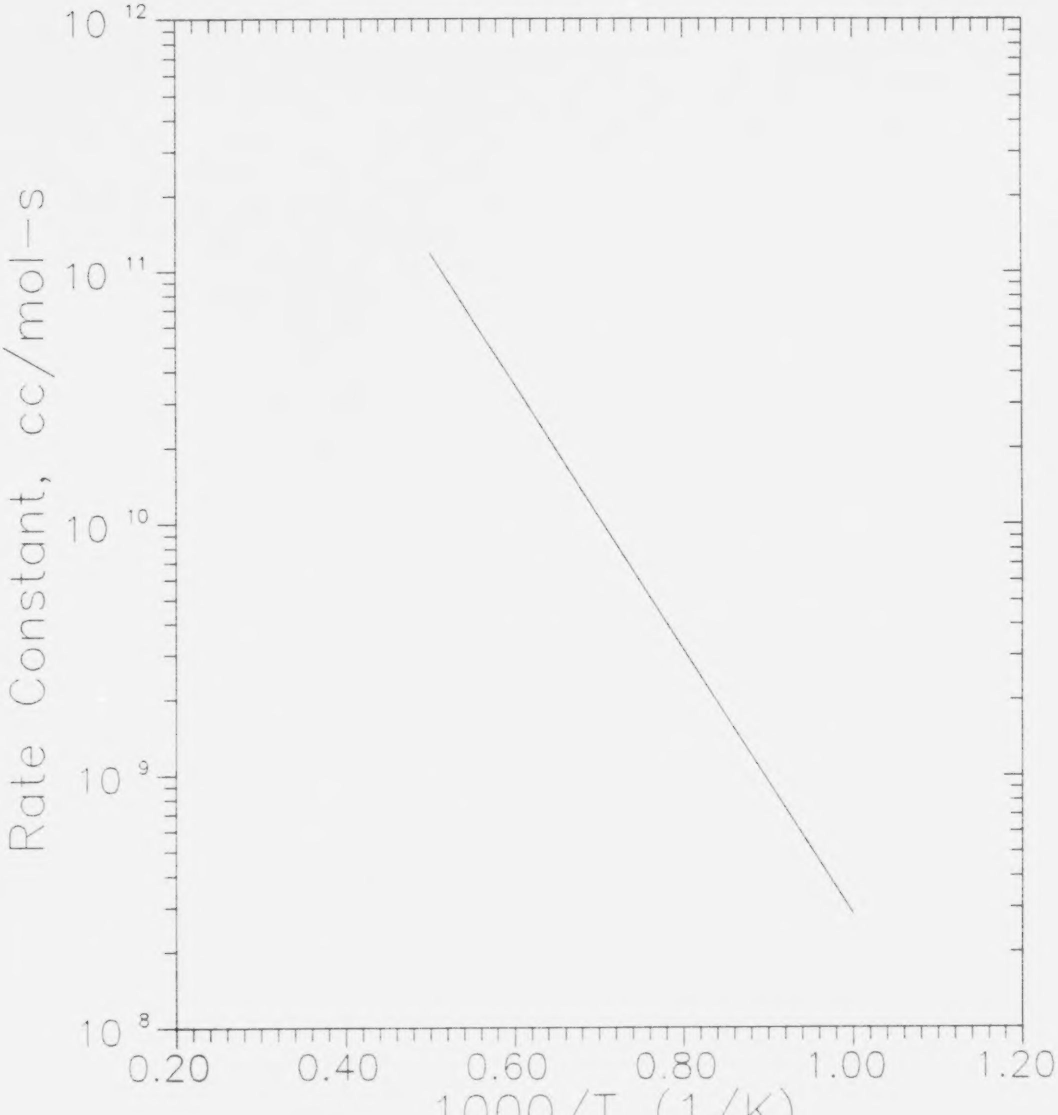
**CH4 + CH2 = CH3 + CH3**


10 14
10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

$CH_4 + CH = C_2H_4 + H$

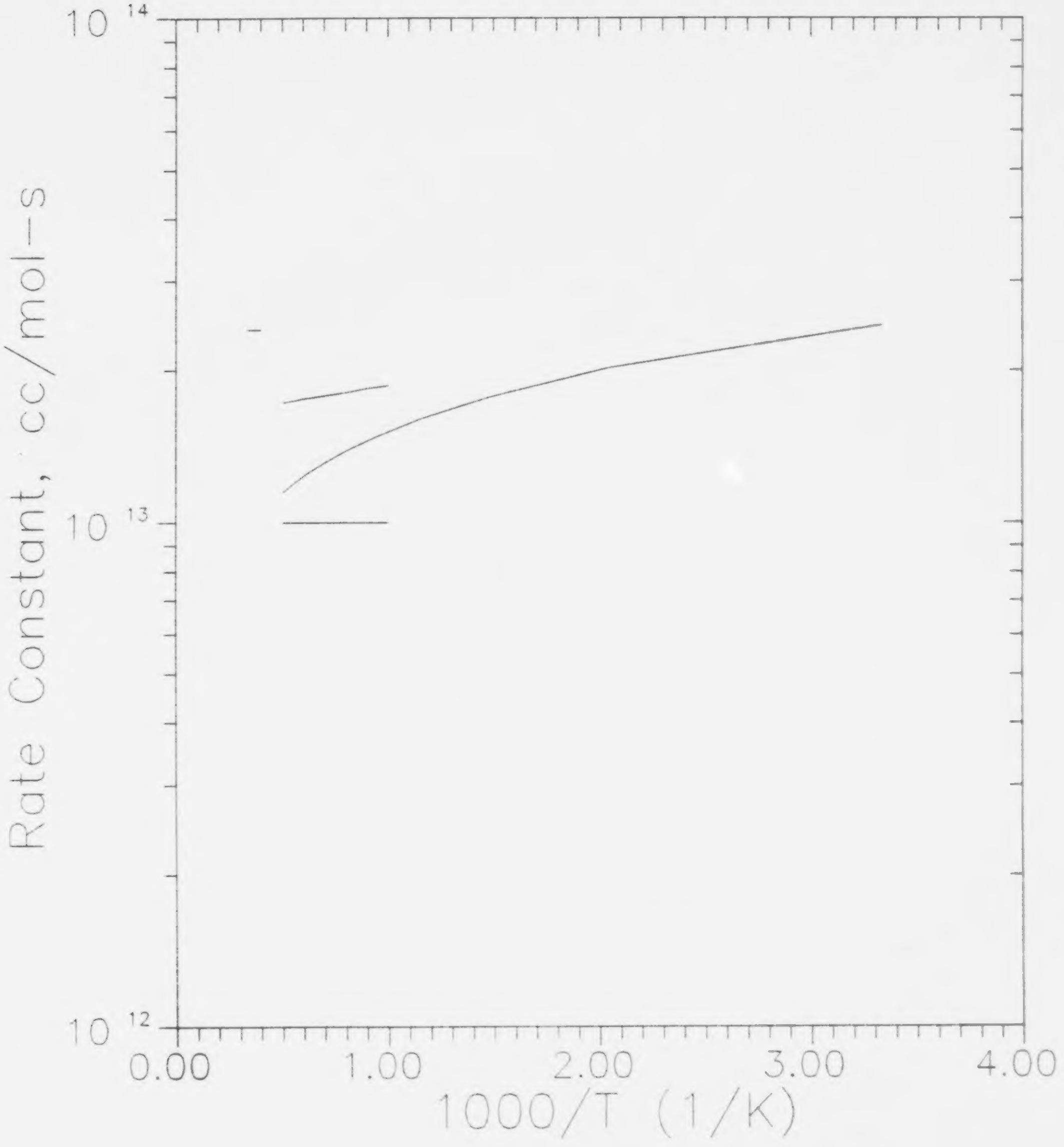


**CH4 + CH = CH3 + CH2**

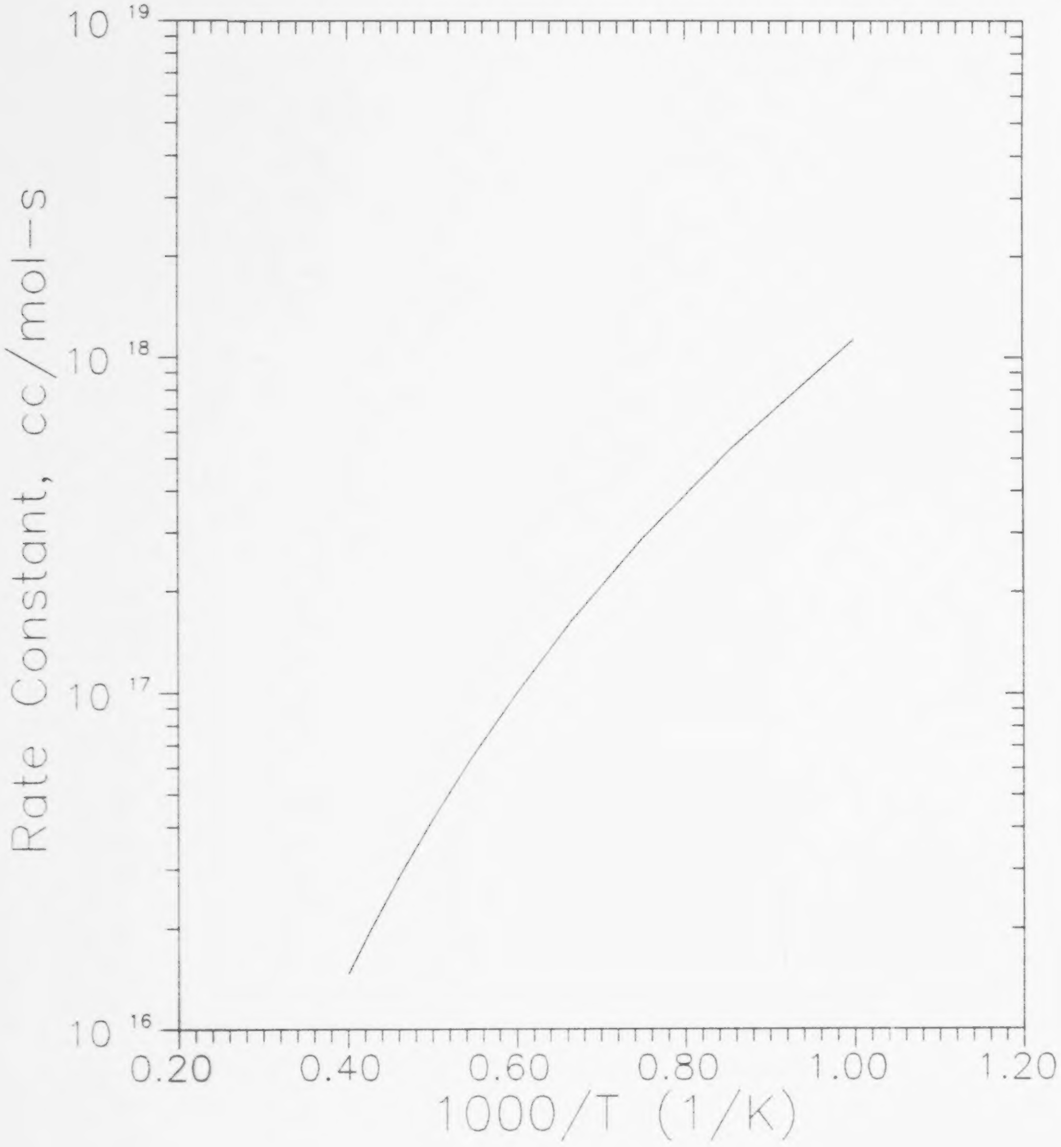


Rate Constant, cc/mol-s
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
$10^{8}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

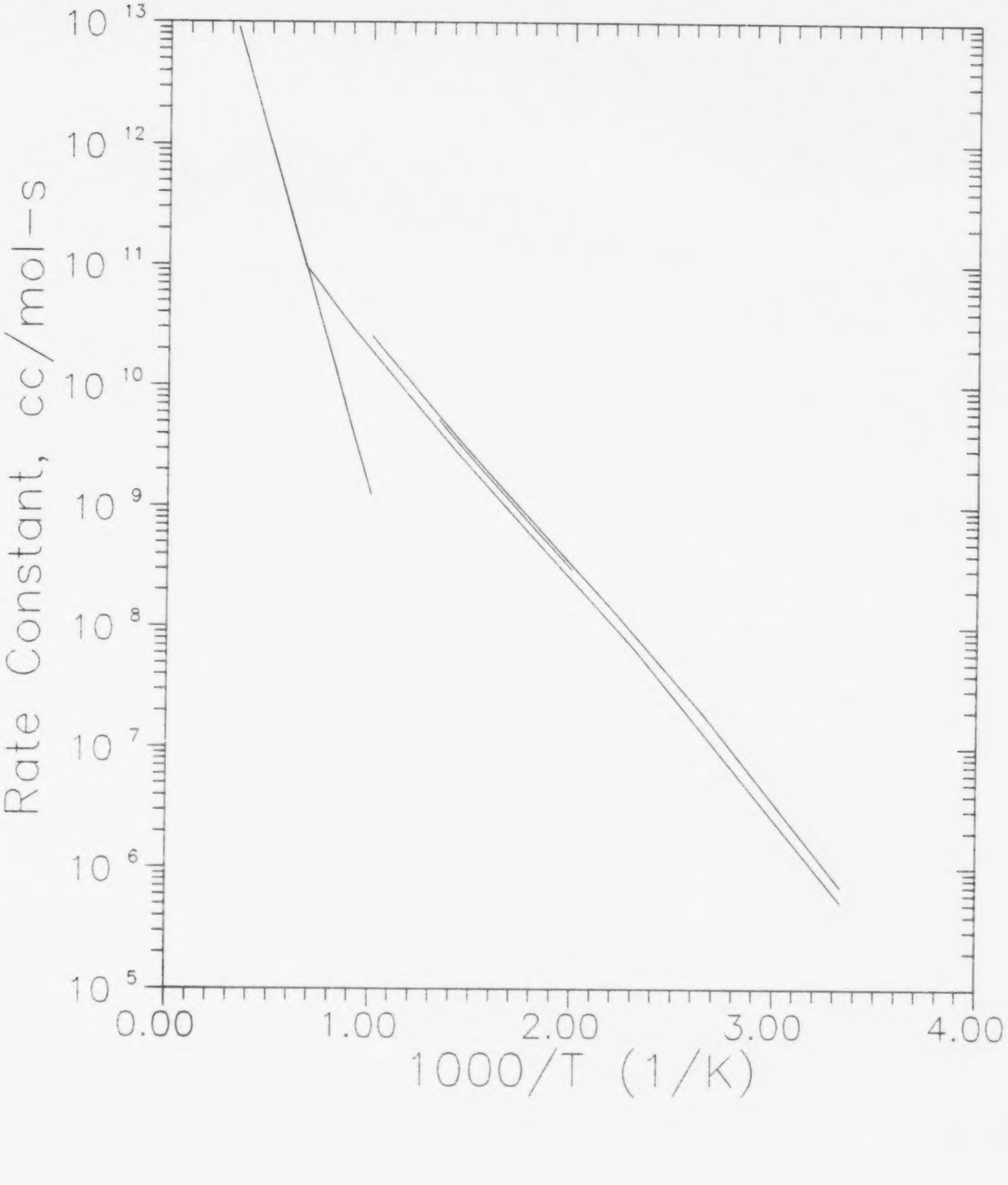
**CH4 + C = CH + CH3**


10 14
10 13
10 12
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

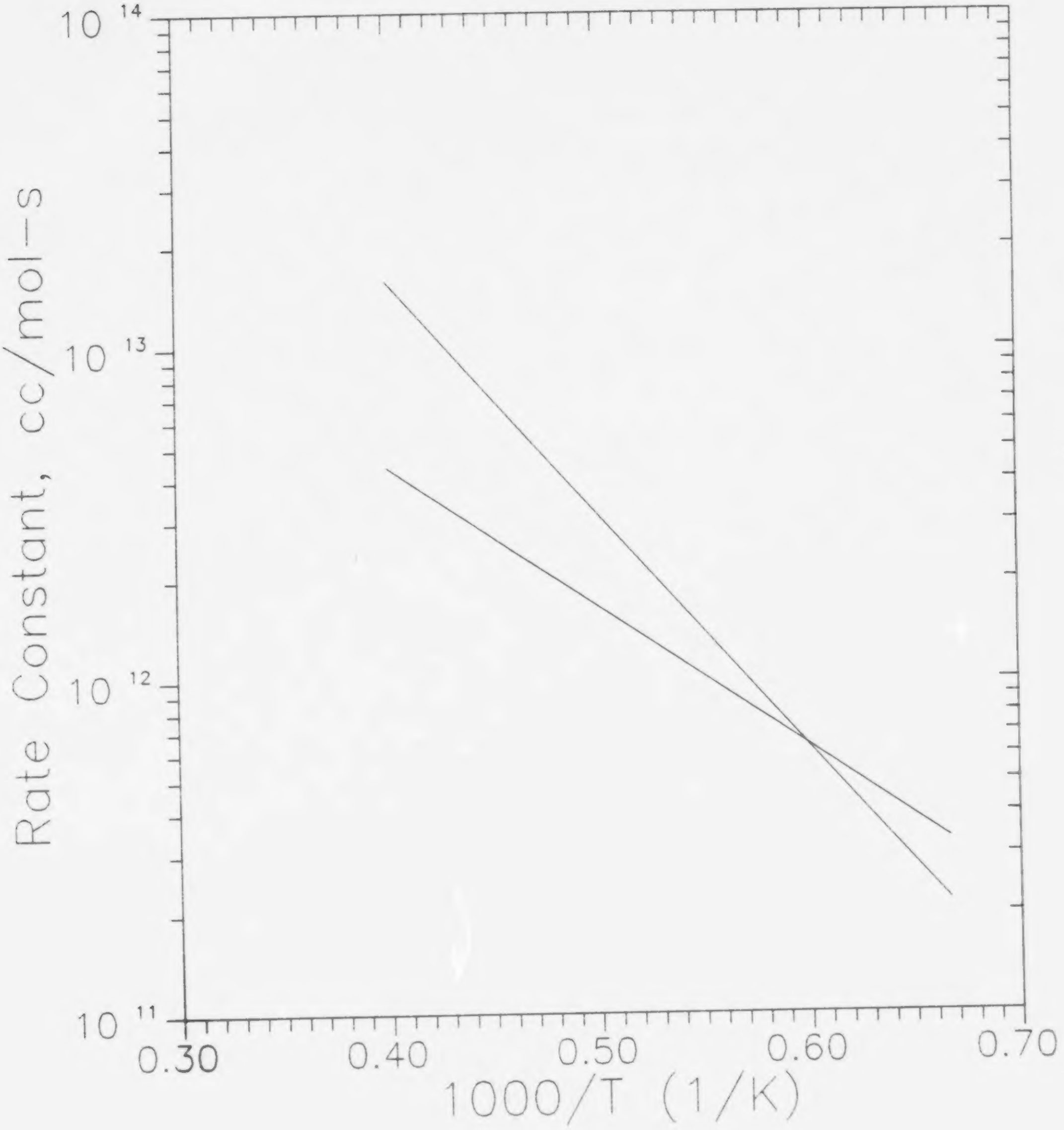
**CH3 + CH3 = C2H6**



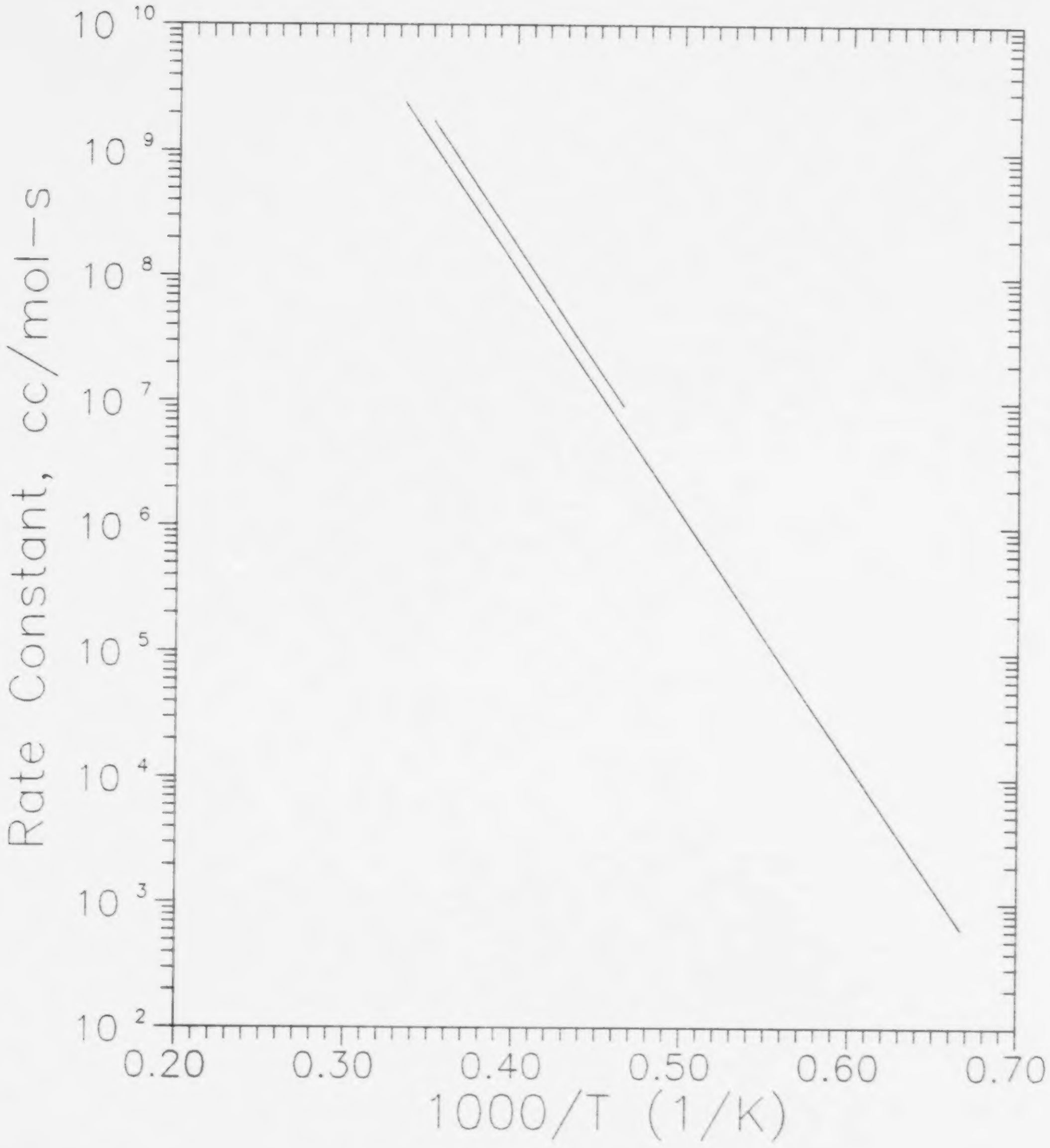
**CH3 + CH3 + M = C2H6 + M**



**$CH_3$ + $CH_3$ = $C_2H_5$ + H**

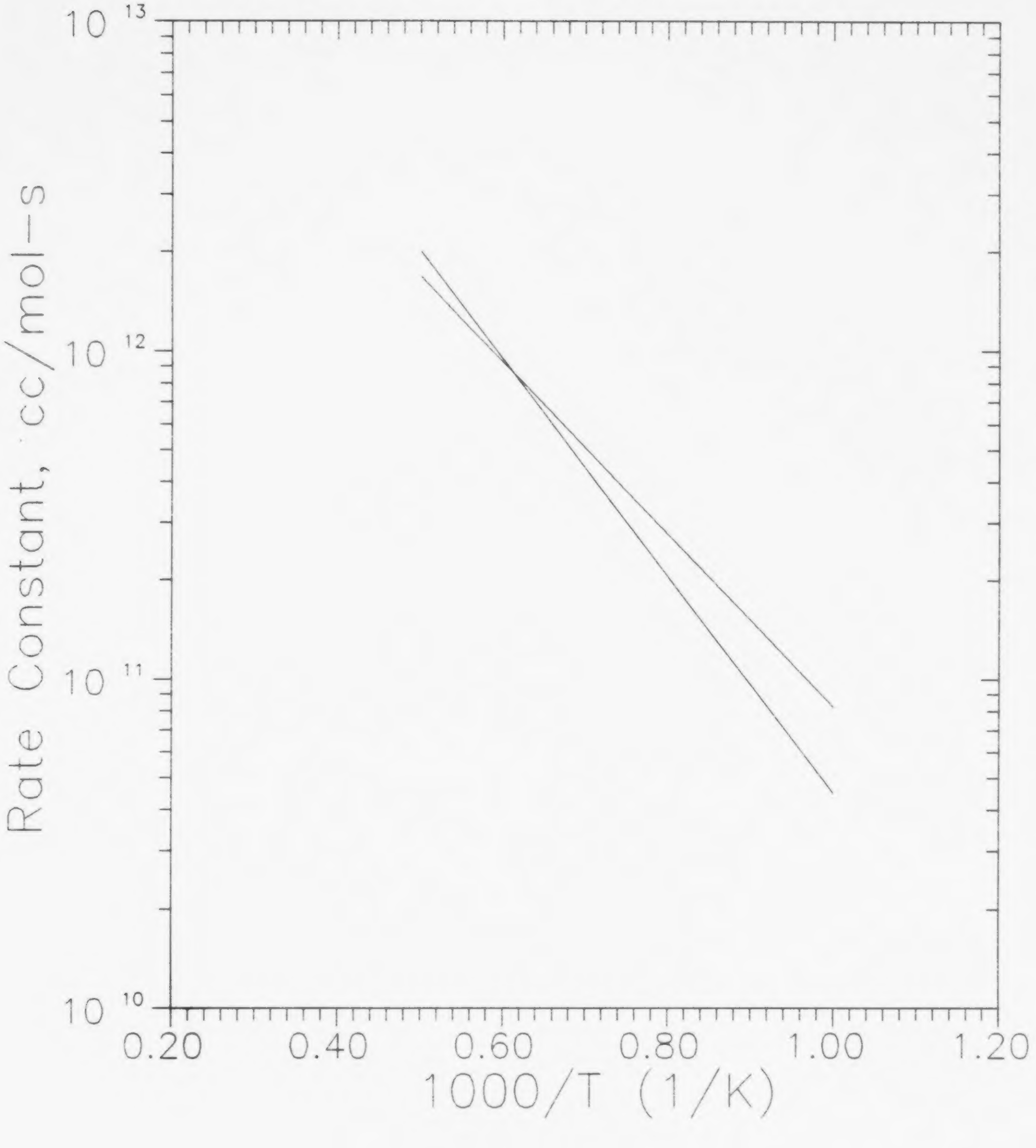


**CH3 + CH3 = C2H4 + H2**



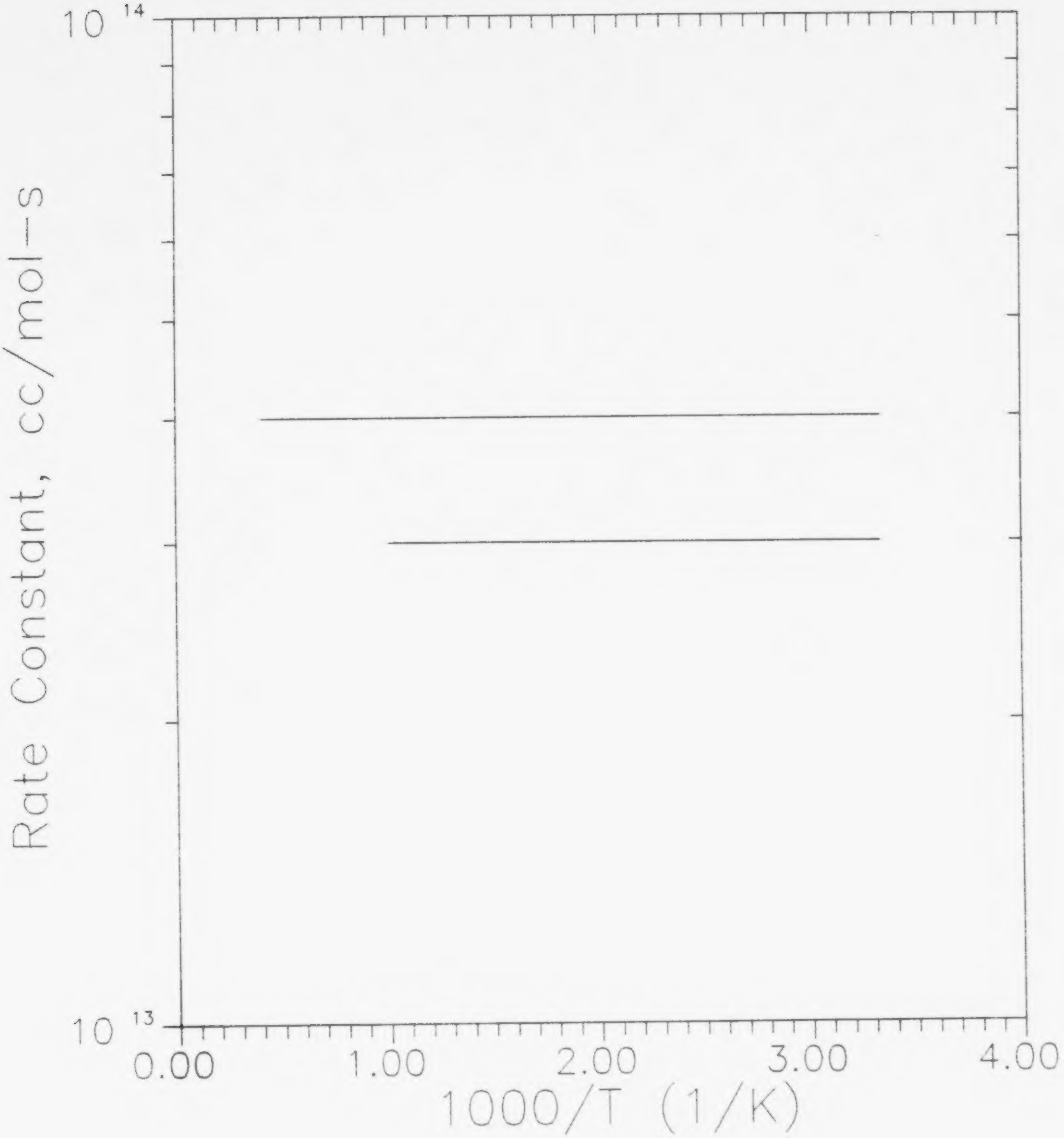
Rate Constant, cc/mol-s
$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
$10^{5}$
$10^{4}$
$10^{3}$
$10^{2}$
0.20
0.30
0.40
0.50
0.60
0.70
1000/T (1/K)

**CH3 + M = CH2 + H + M**

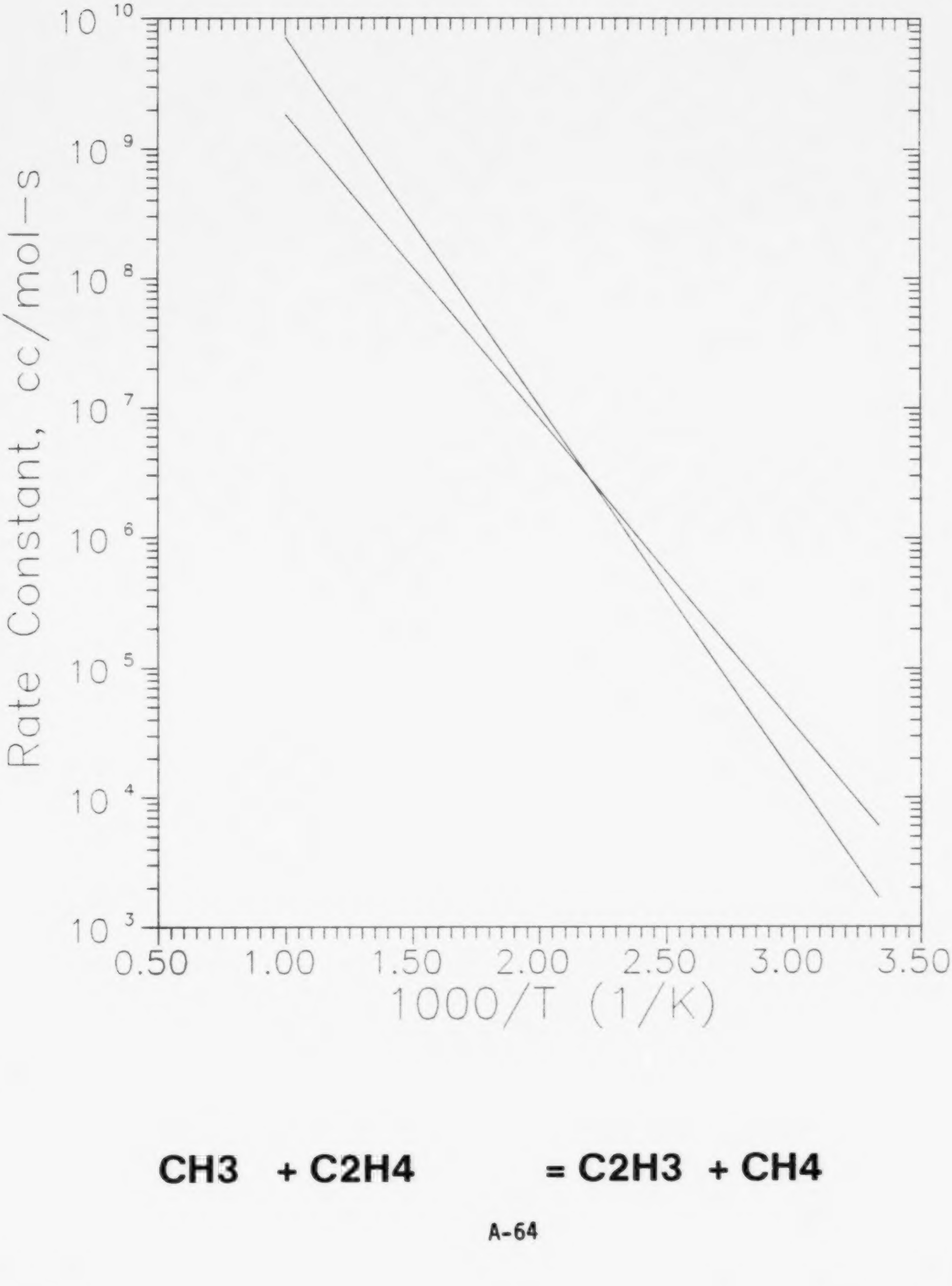


10 13
10 12
10 11
10 10
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

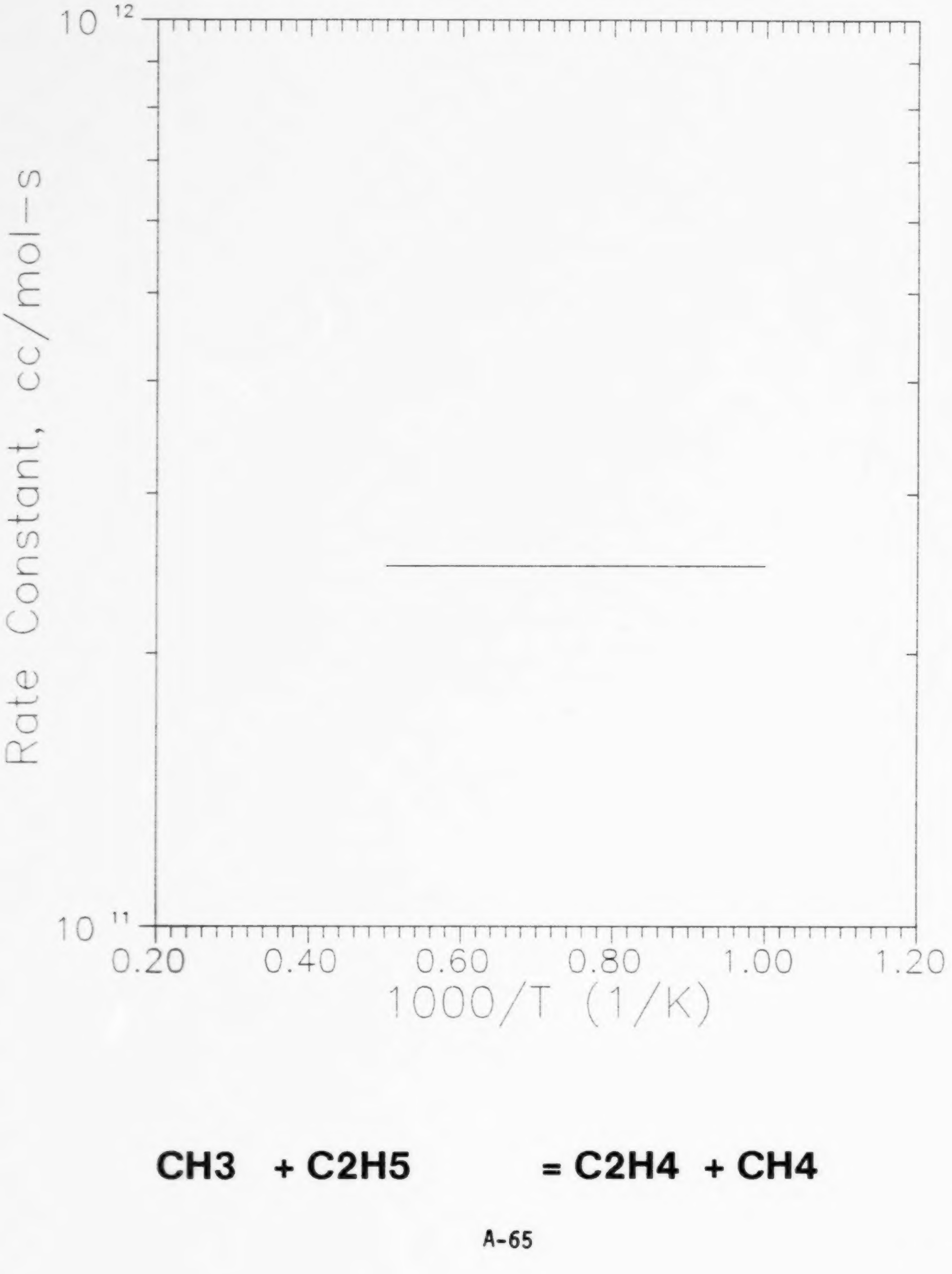
**$CH_3$ + H = $CH_2$ + $H_2$**



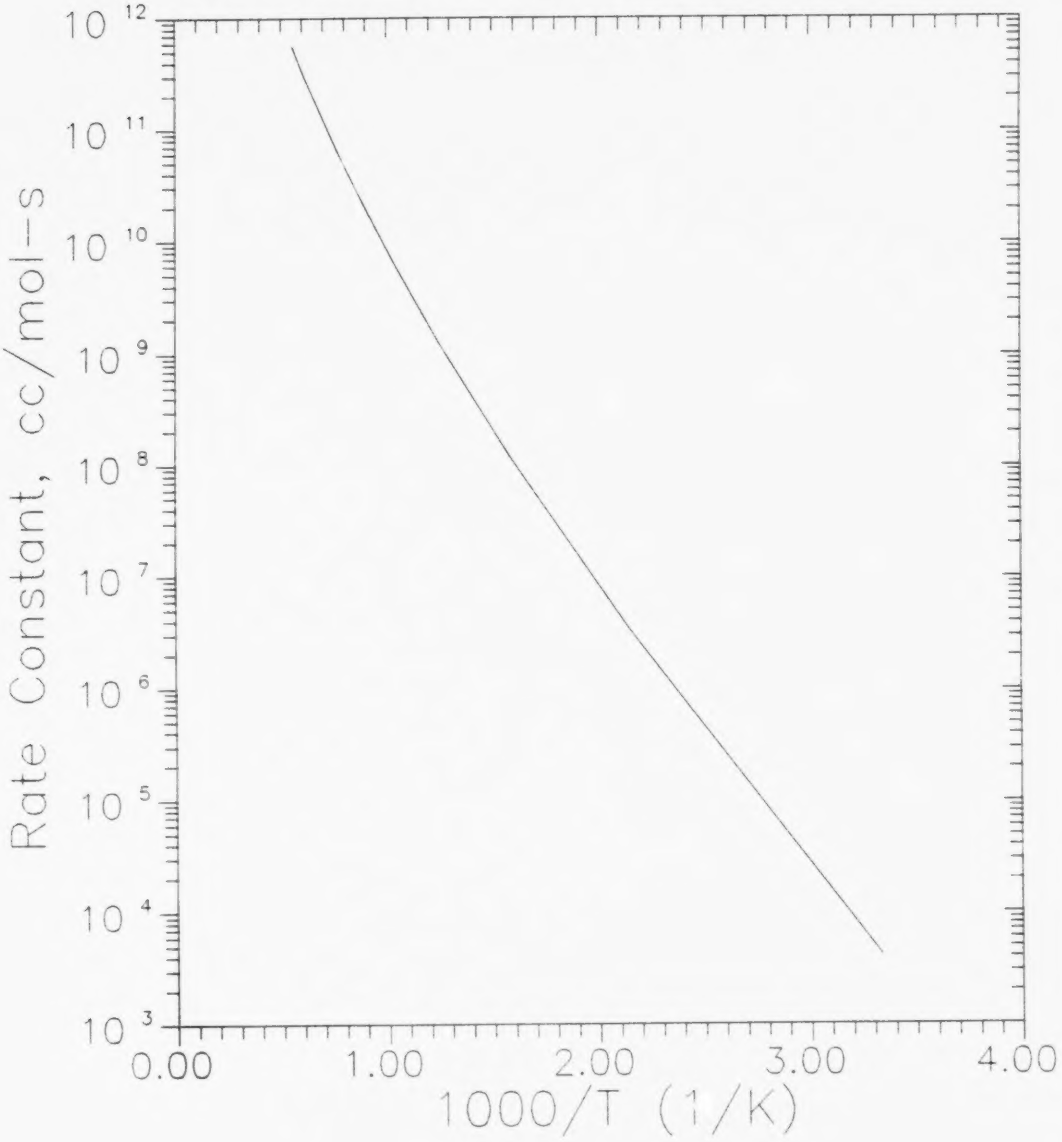
**CH3 + CH2 = C2H4 + H**



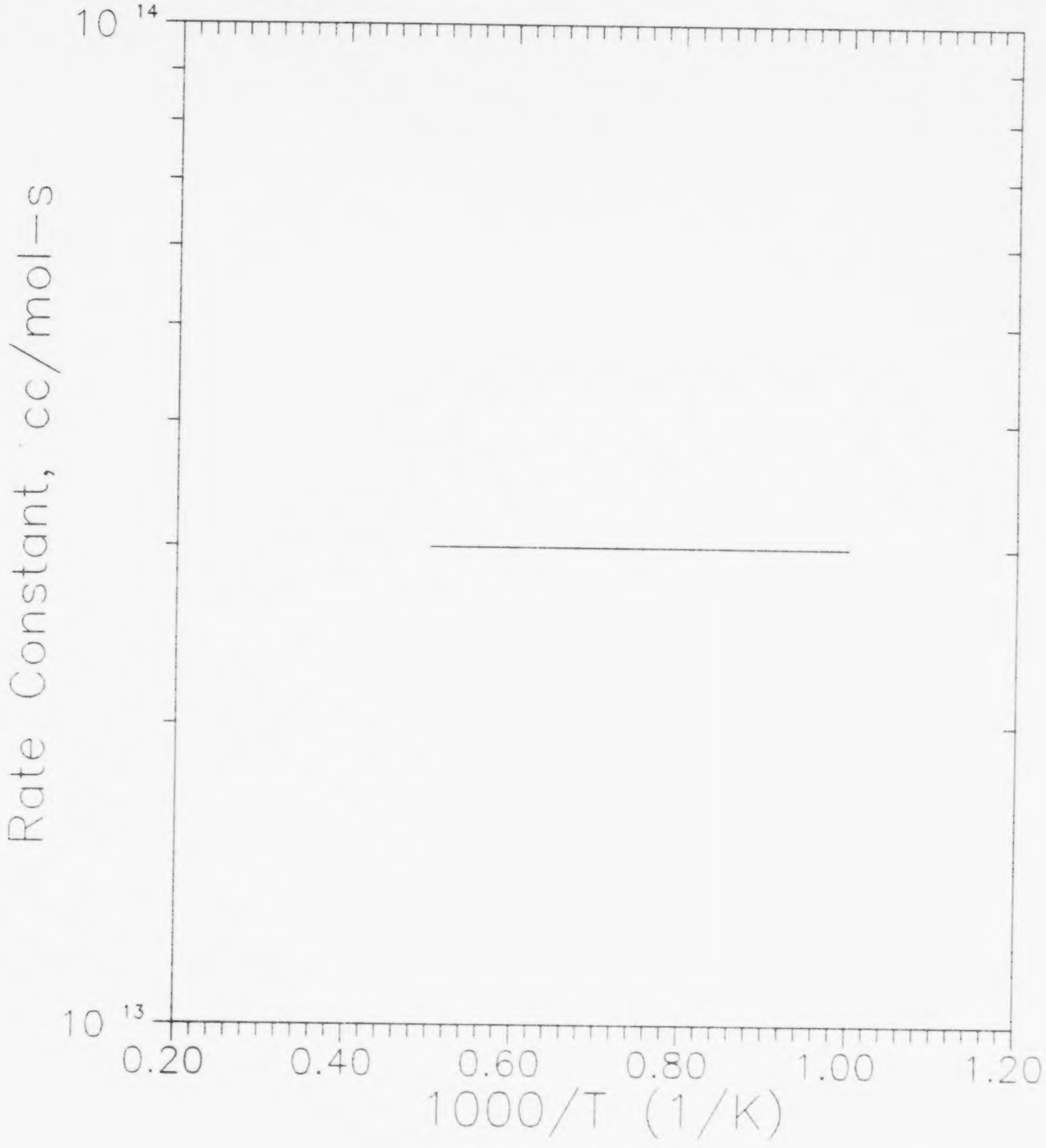
**$CH_3 + C_2H_4 = C_2H_3 + CH_4$**



**CH3 + C2H5 = C2H4 + CH4**

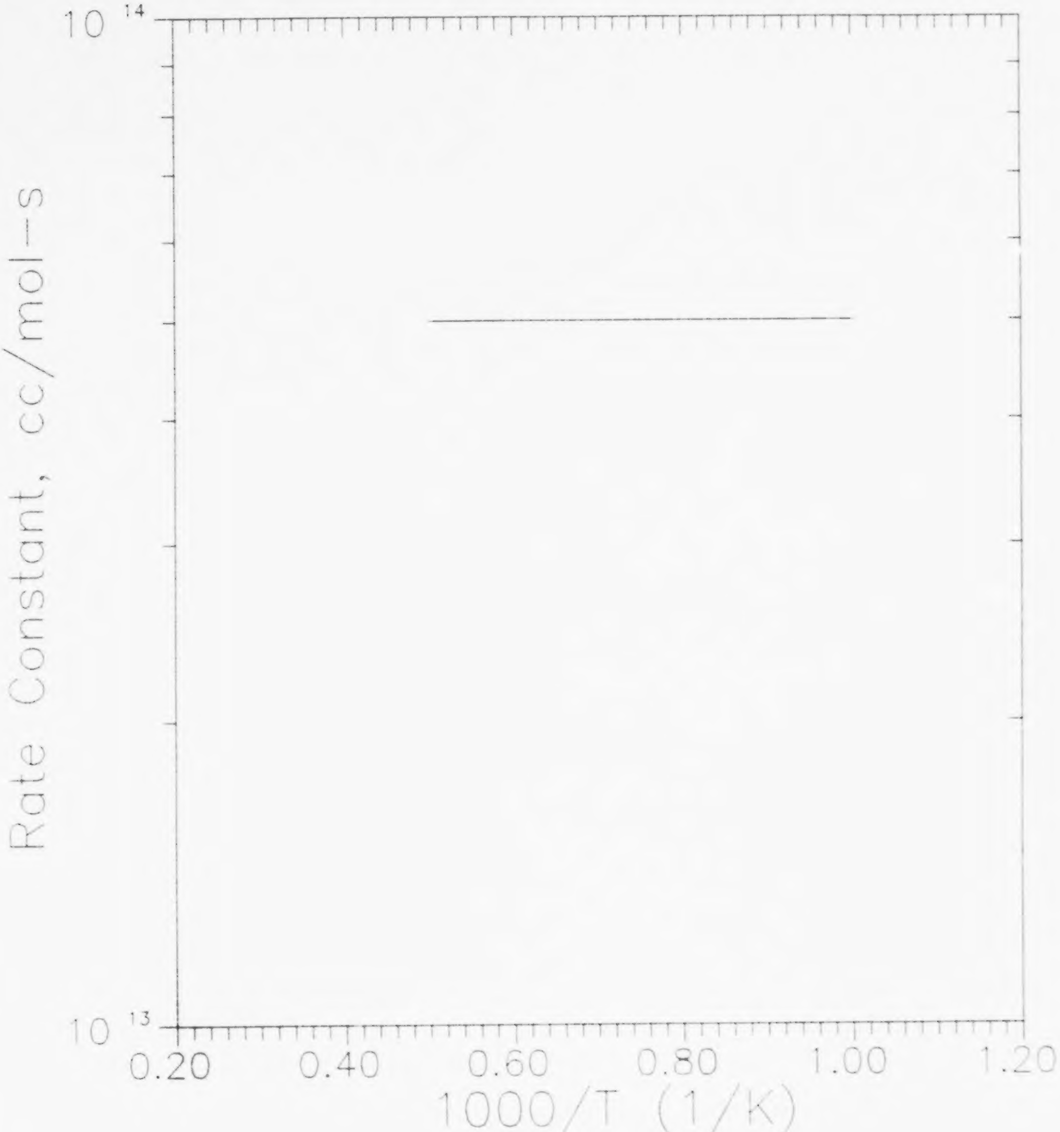


**CH3 + C2H6 = C2H5 + CH4**

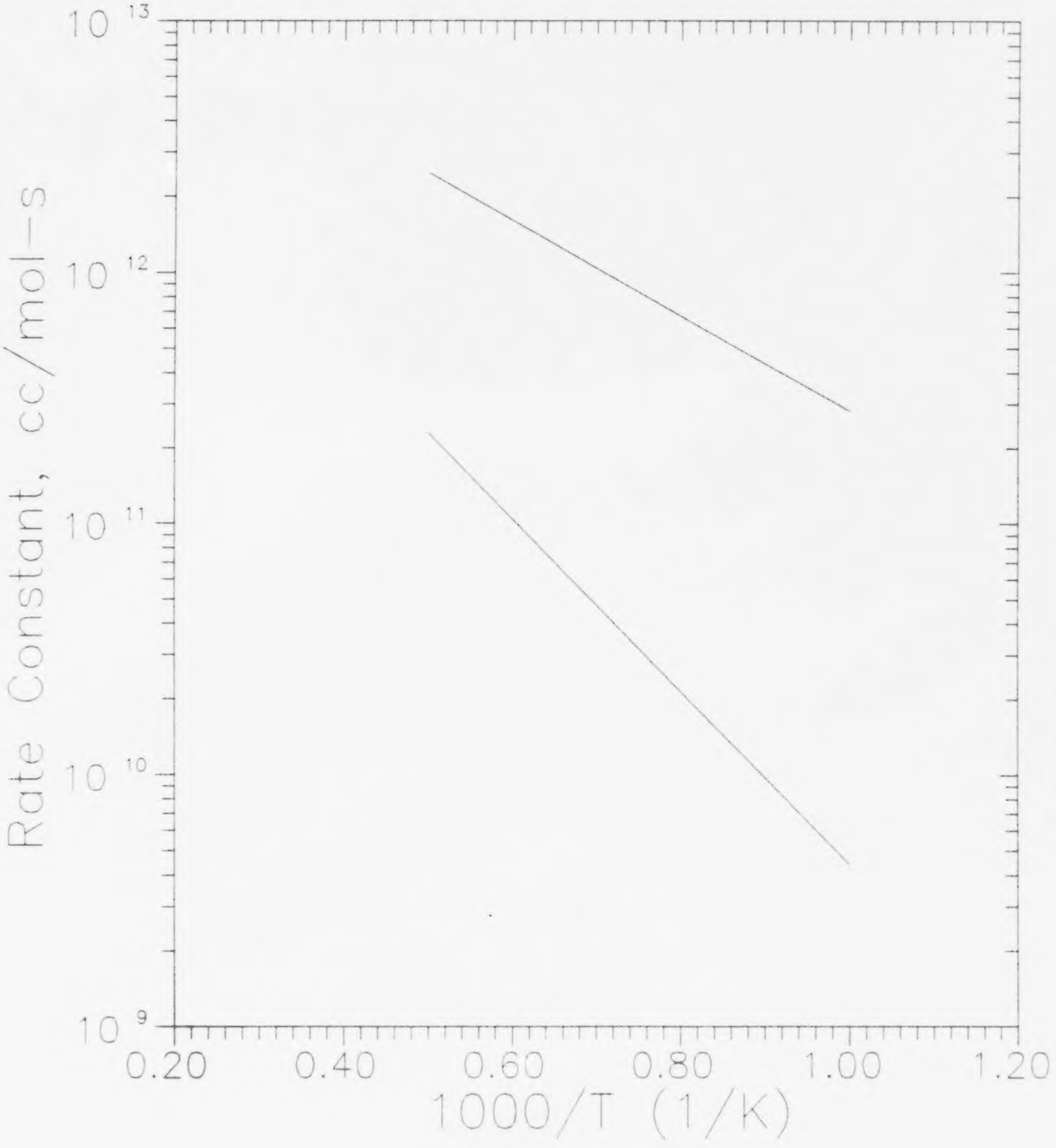


$10^{14}$
$10^{13}$
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

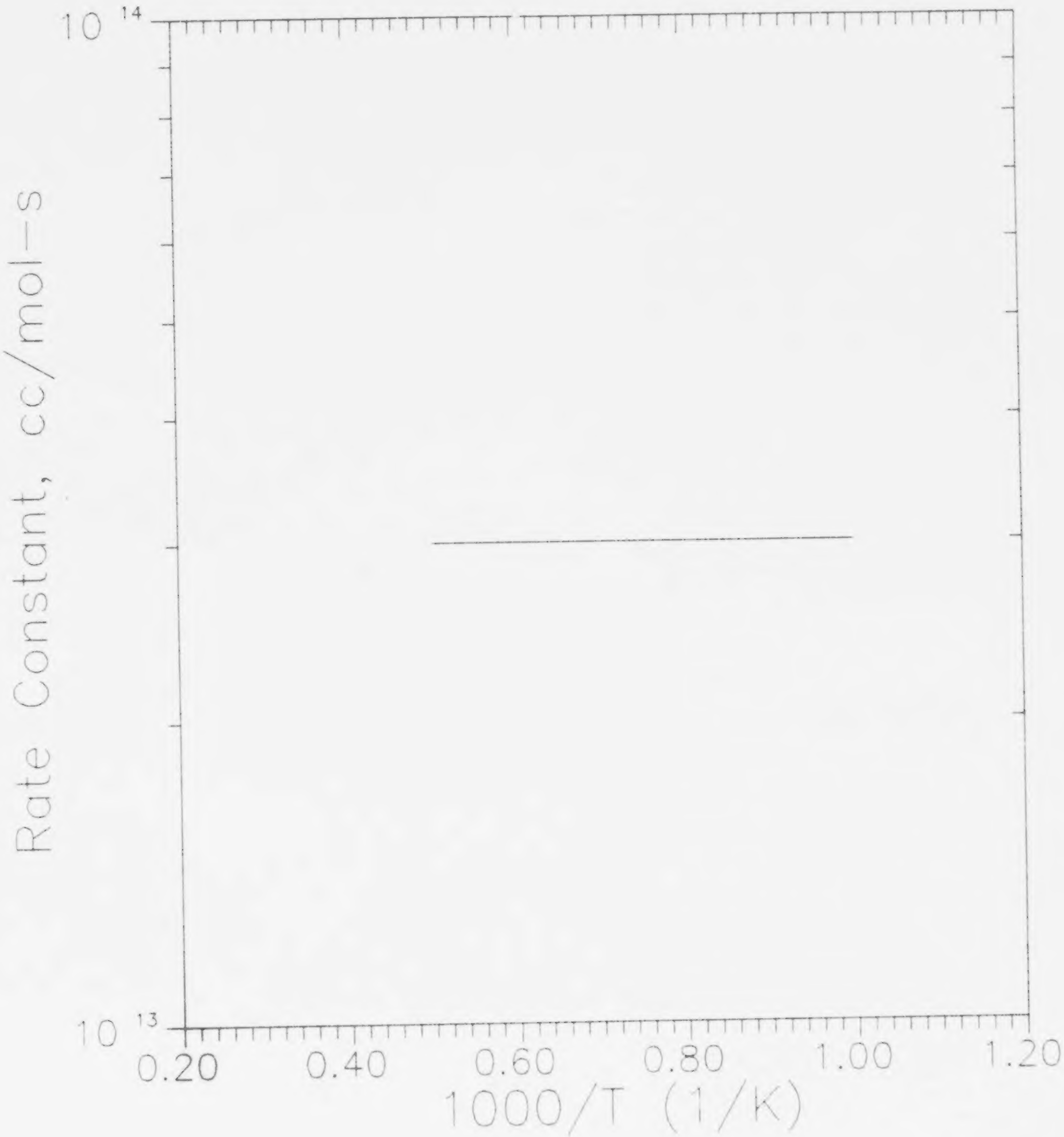
**CH3 + CH = C2H3 + H**


10 14
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

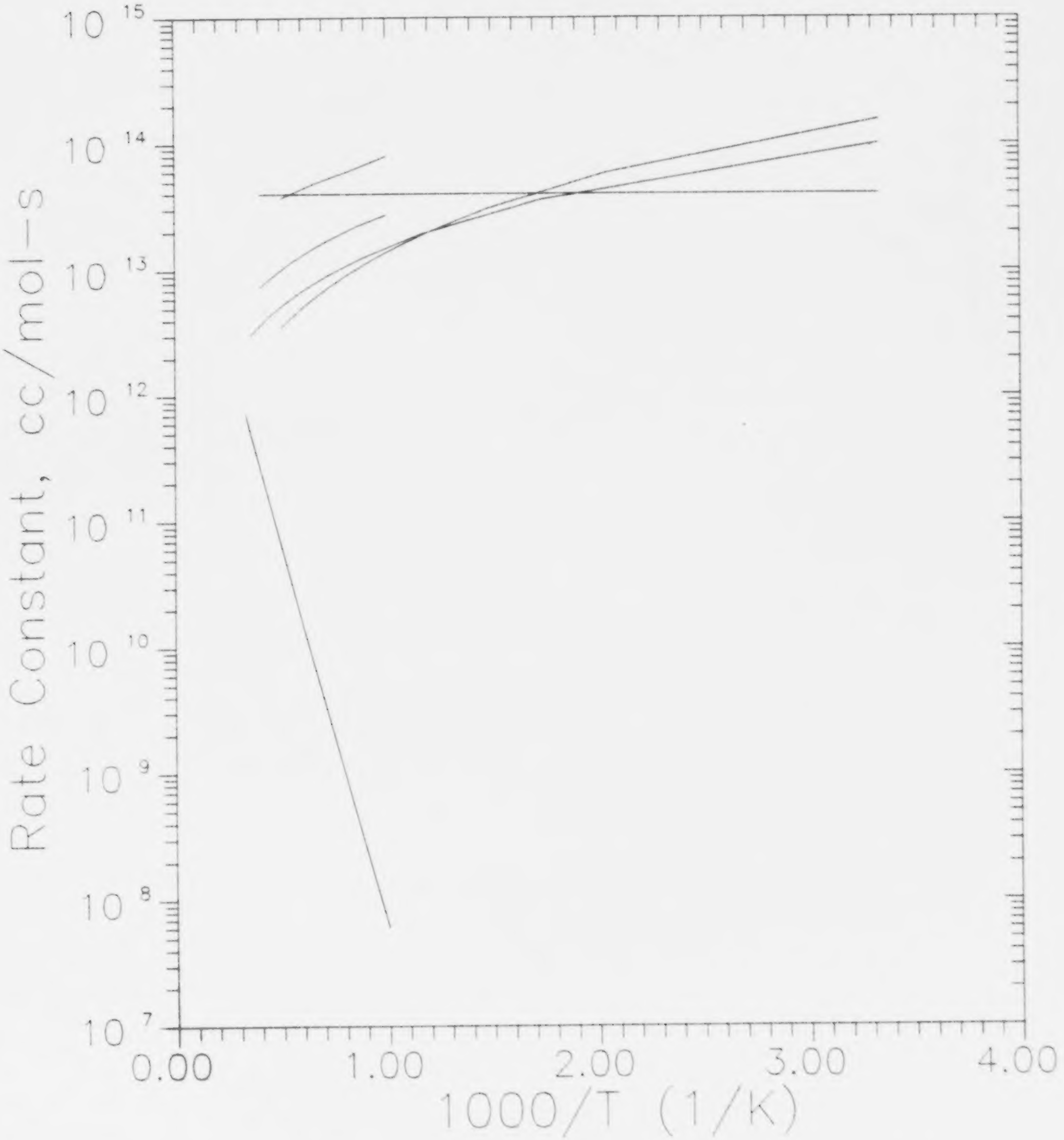
**CH3 + C = C2H2 + H**



CH2 + C2H6 = C2H5 + CH3

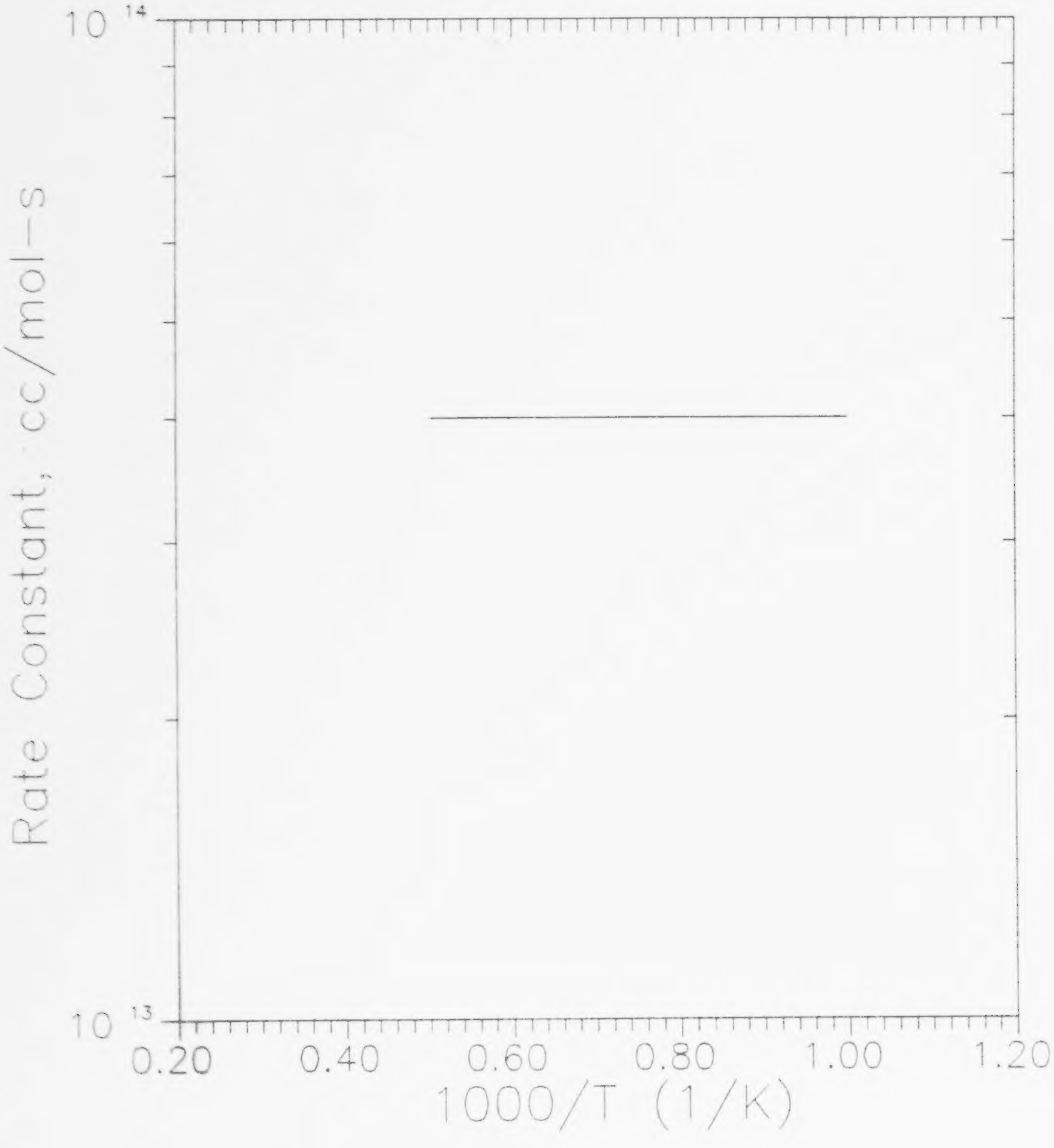


CH2 + C2H3 = C2H2 + CH3

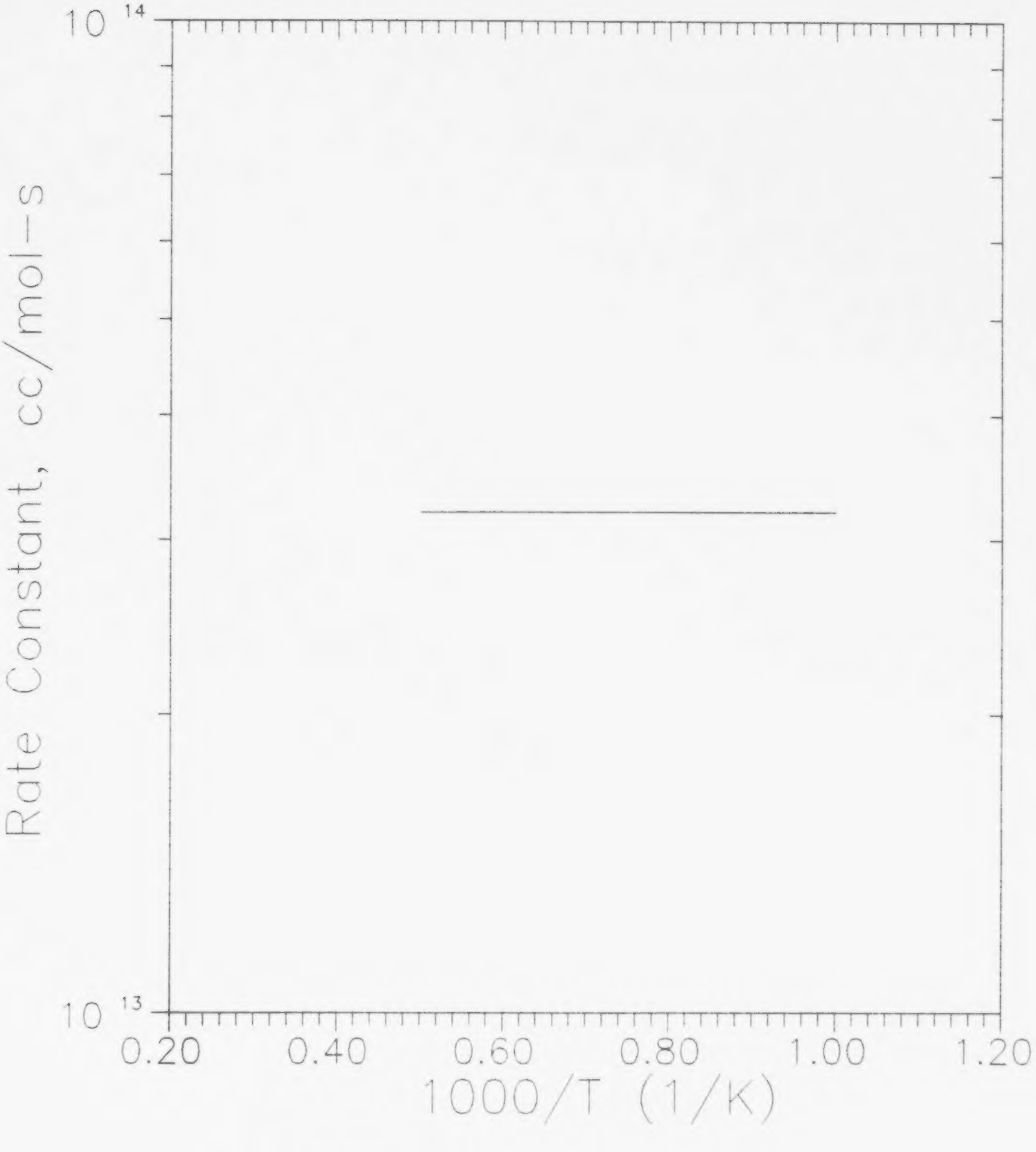


Rate Constant, cc/mol-s
10 15
10 14
10 13
10 12
10 11
10 10
10 9
10 8
10 7
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

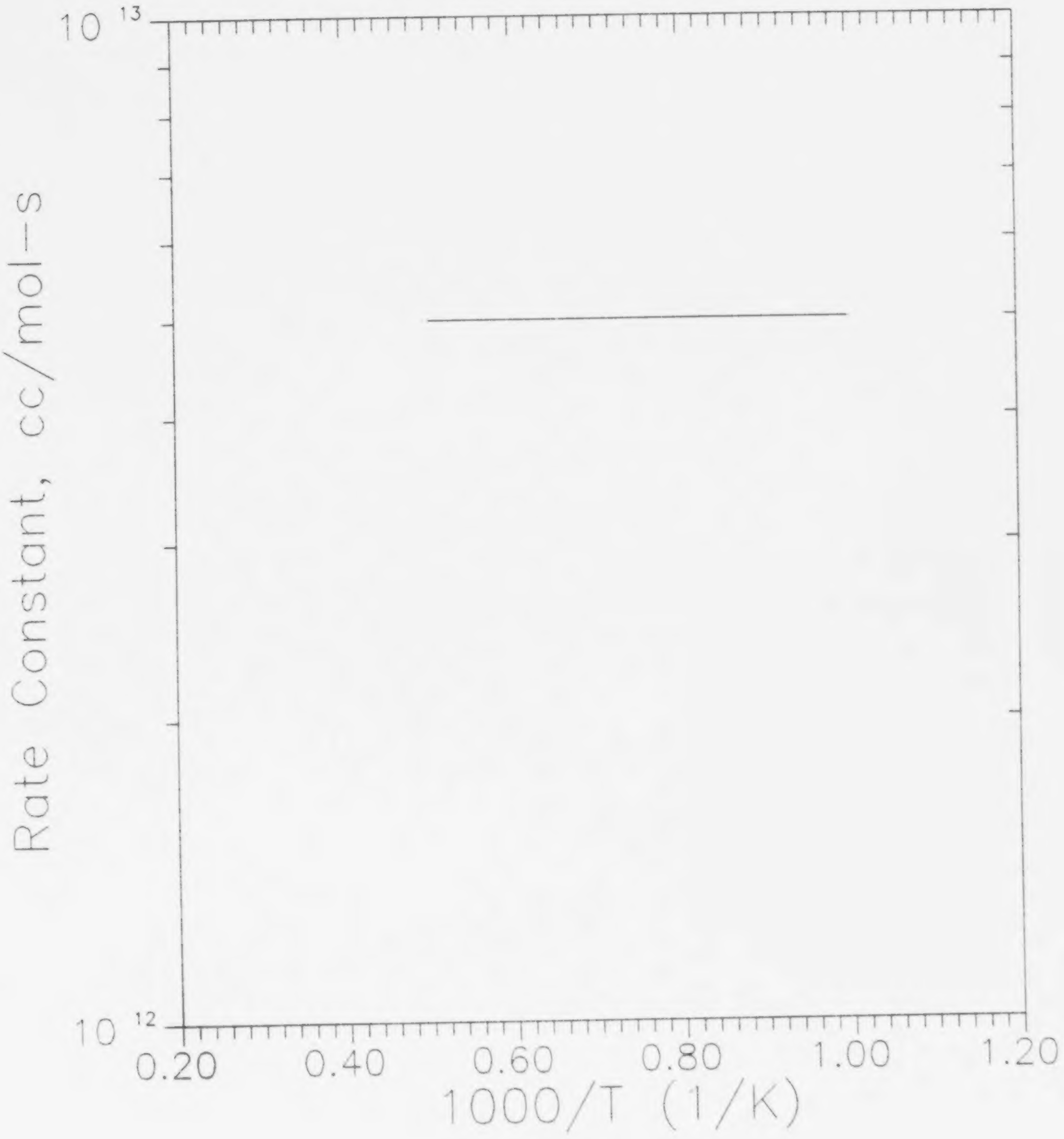
**CH2 + H = CH + H2**


10 14
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

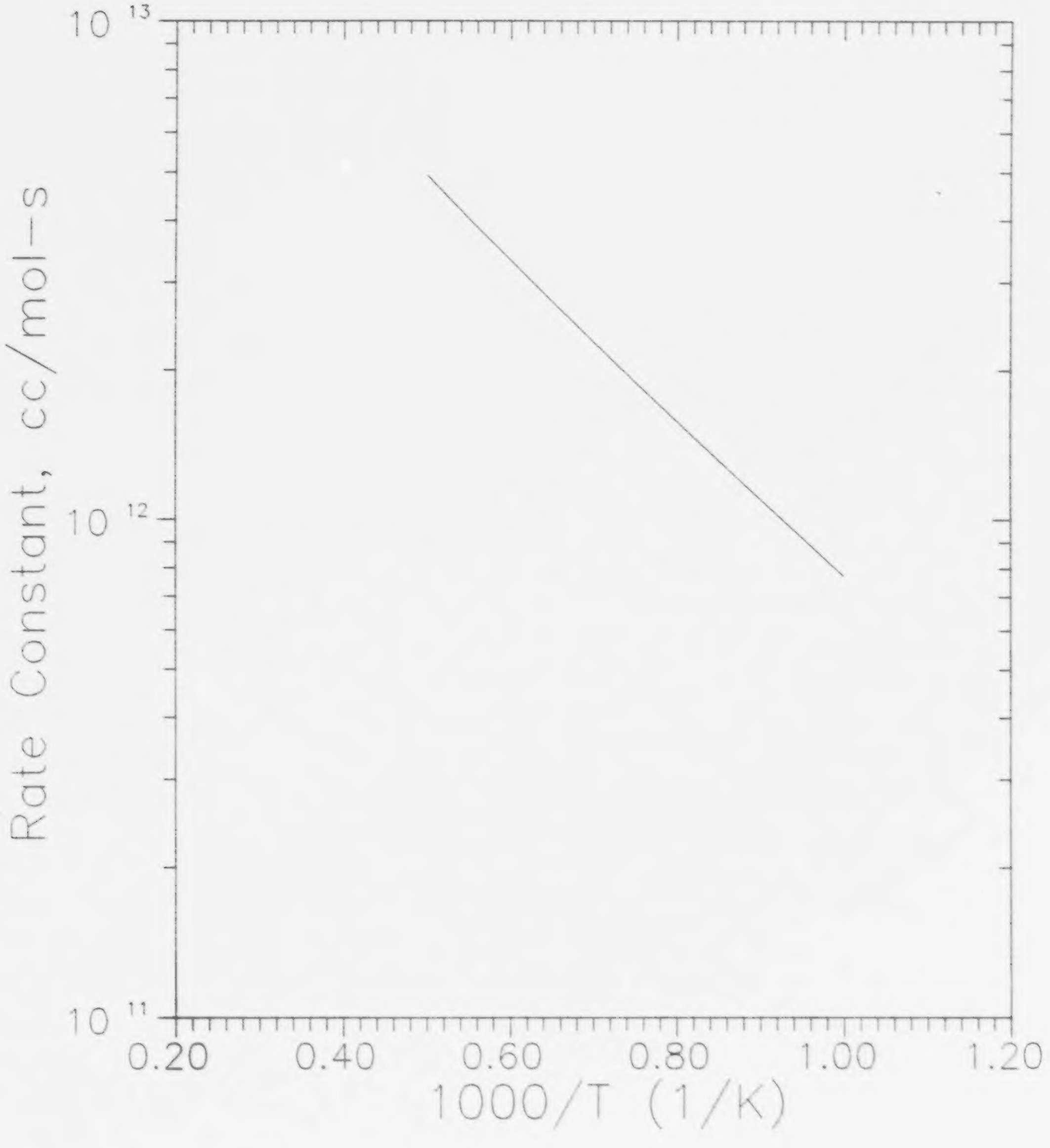
**CH2 + CH = C2H2 + H**



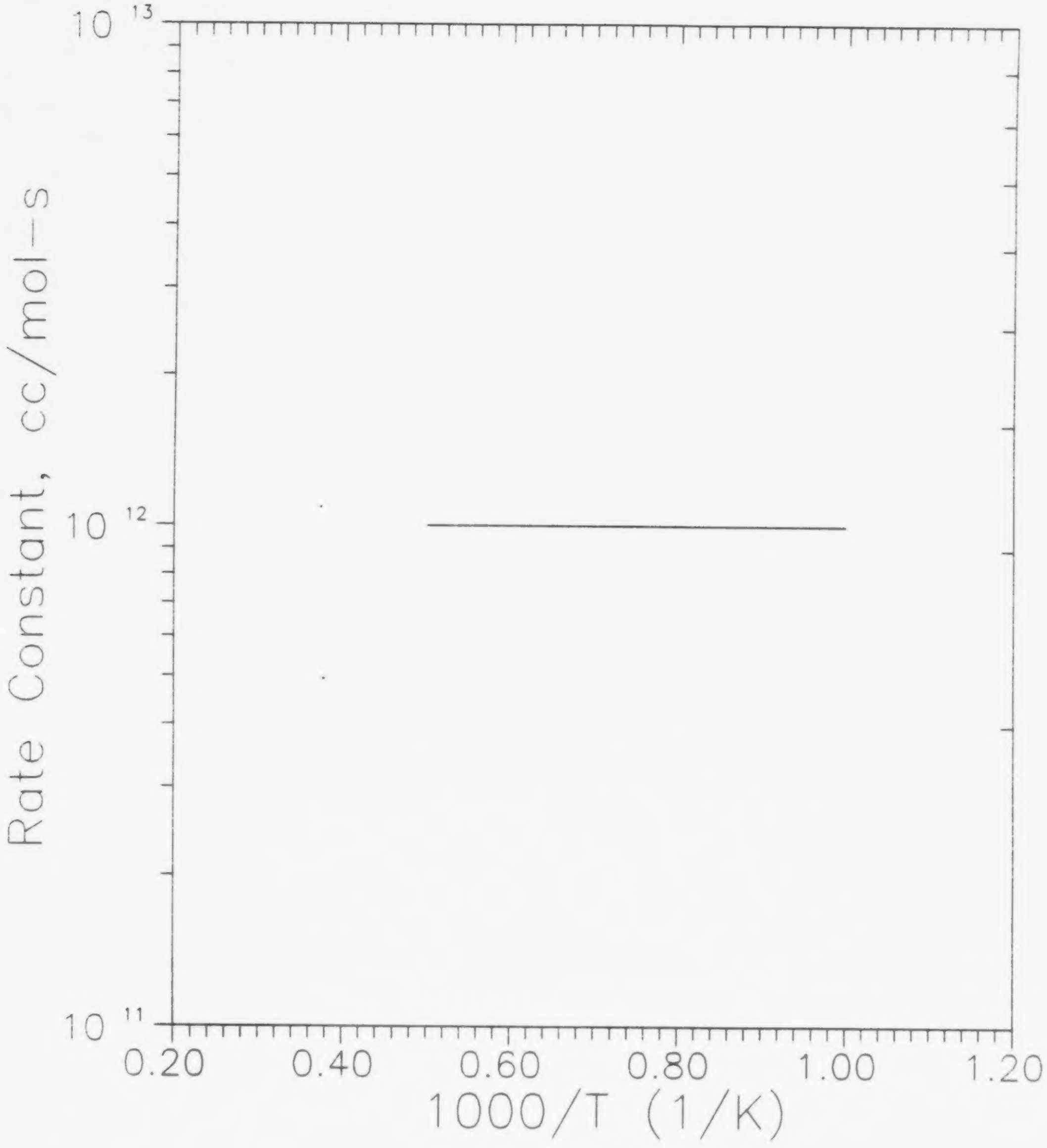
**CH2 + CH2 = C2H2 + H2**



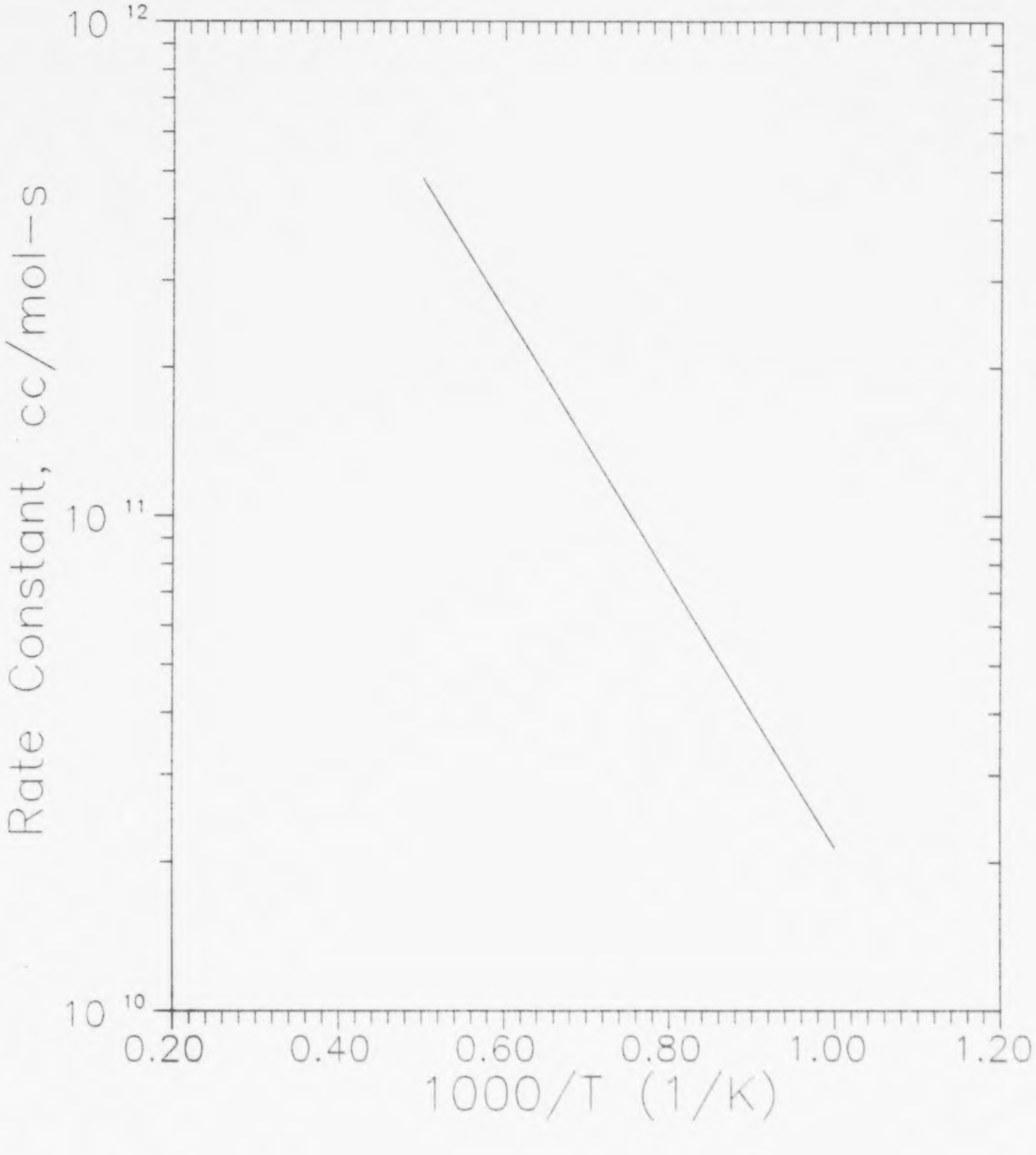
CH2 + CH2 = C2H3 + H



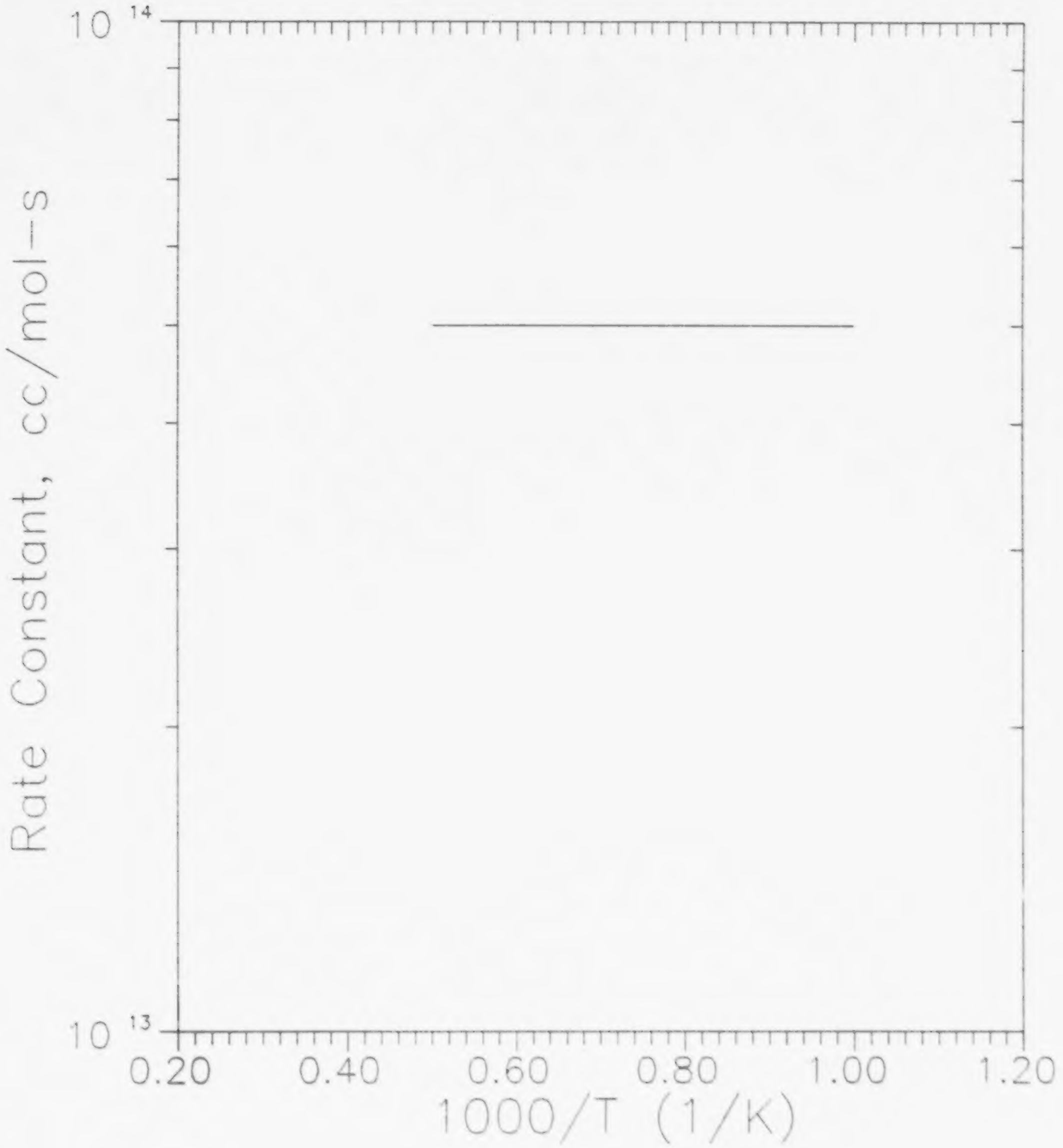
**$CH_2 + CH_2 = CH_3 + CH$**



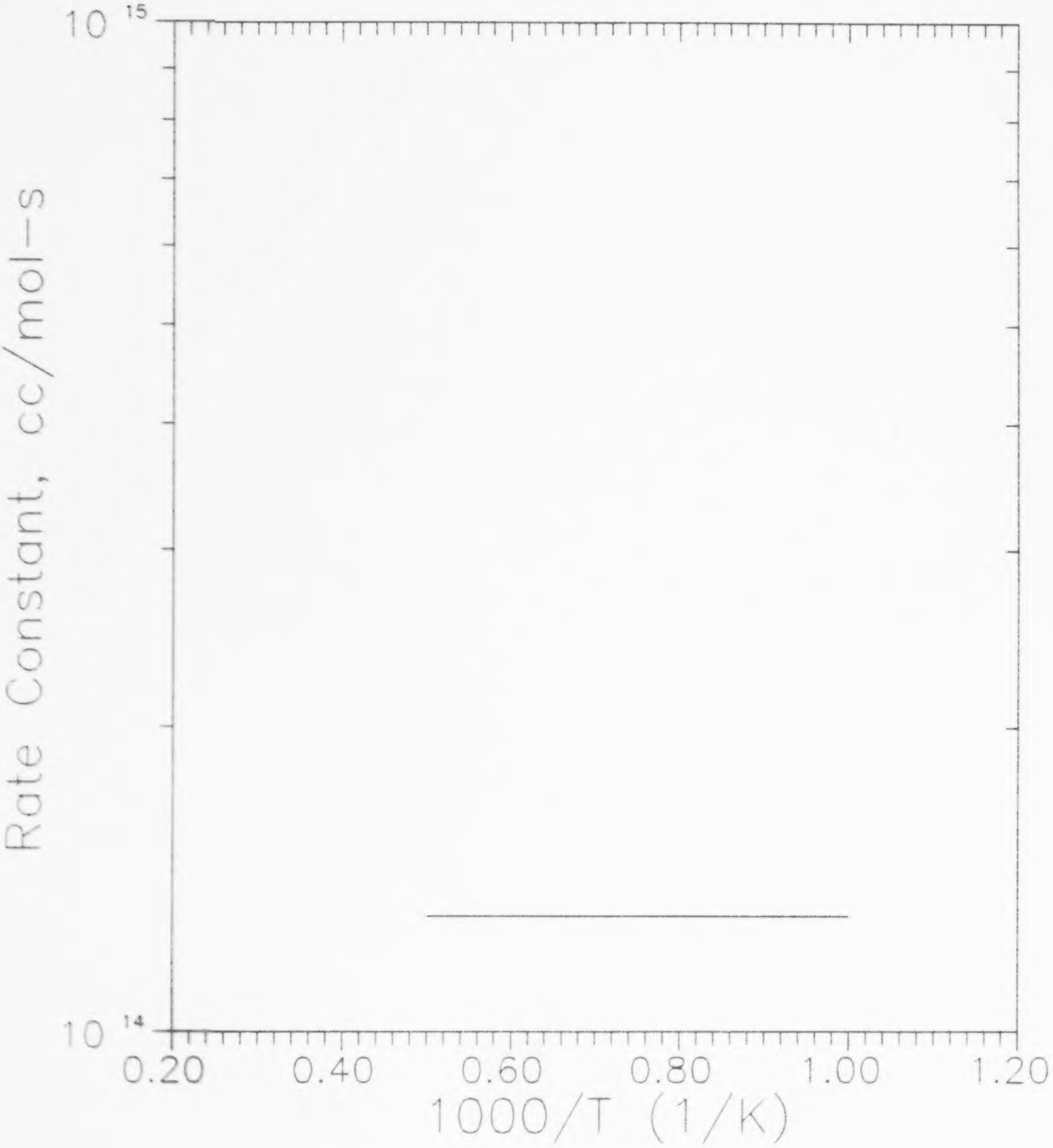
**CH2 + C2H2 = CH3 + C2H**



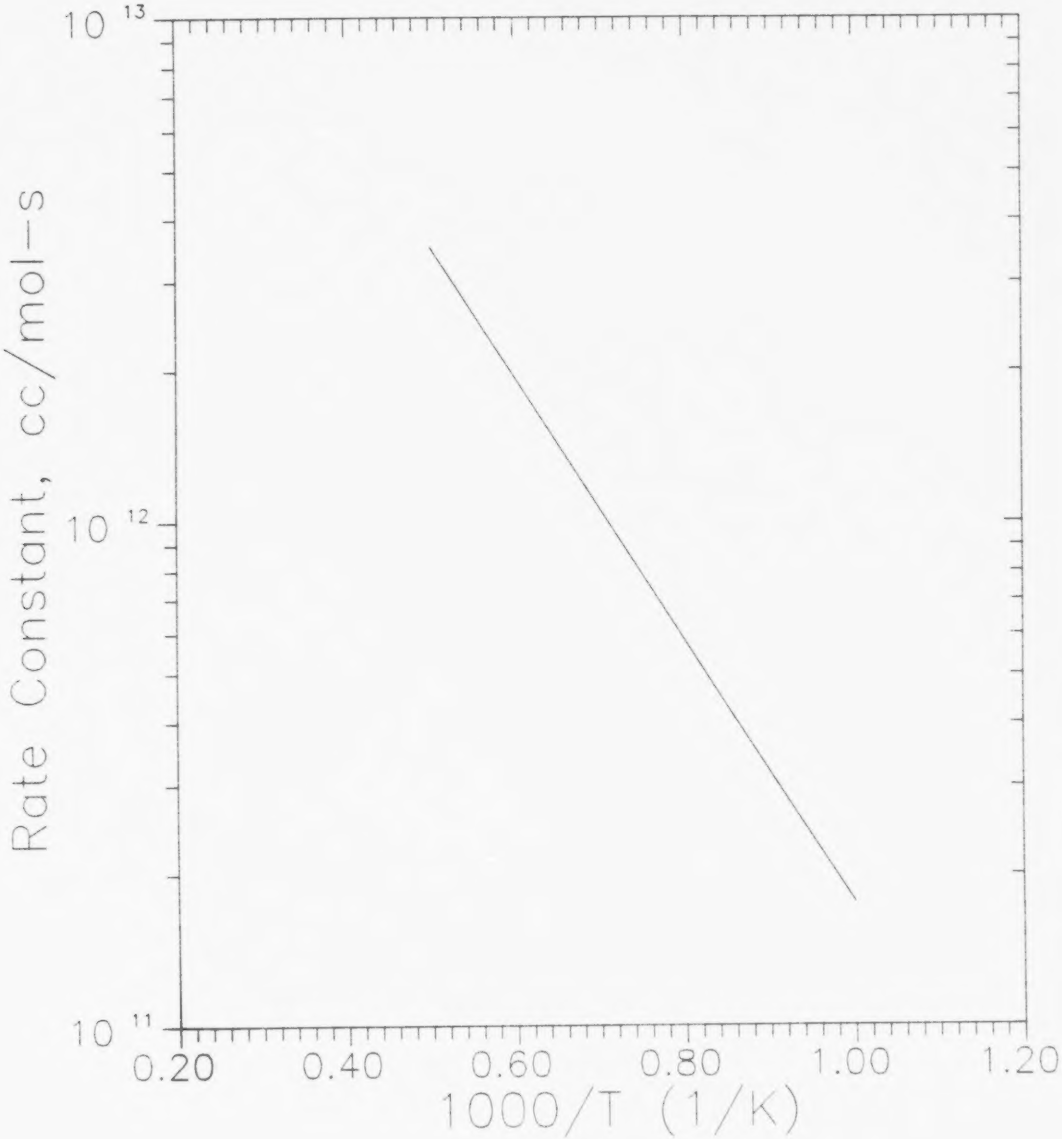
**CH2 + C2H4 = CH3 + C2H3**


10 $^{14}$
10 $^{13}$
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

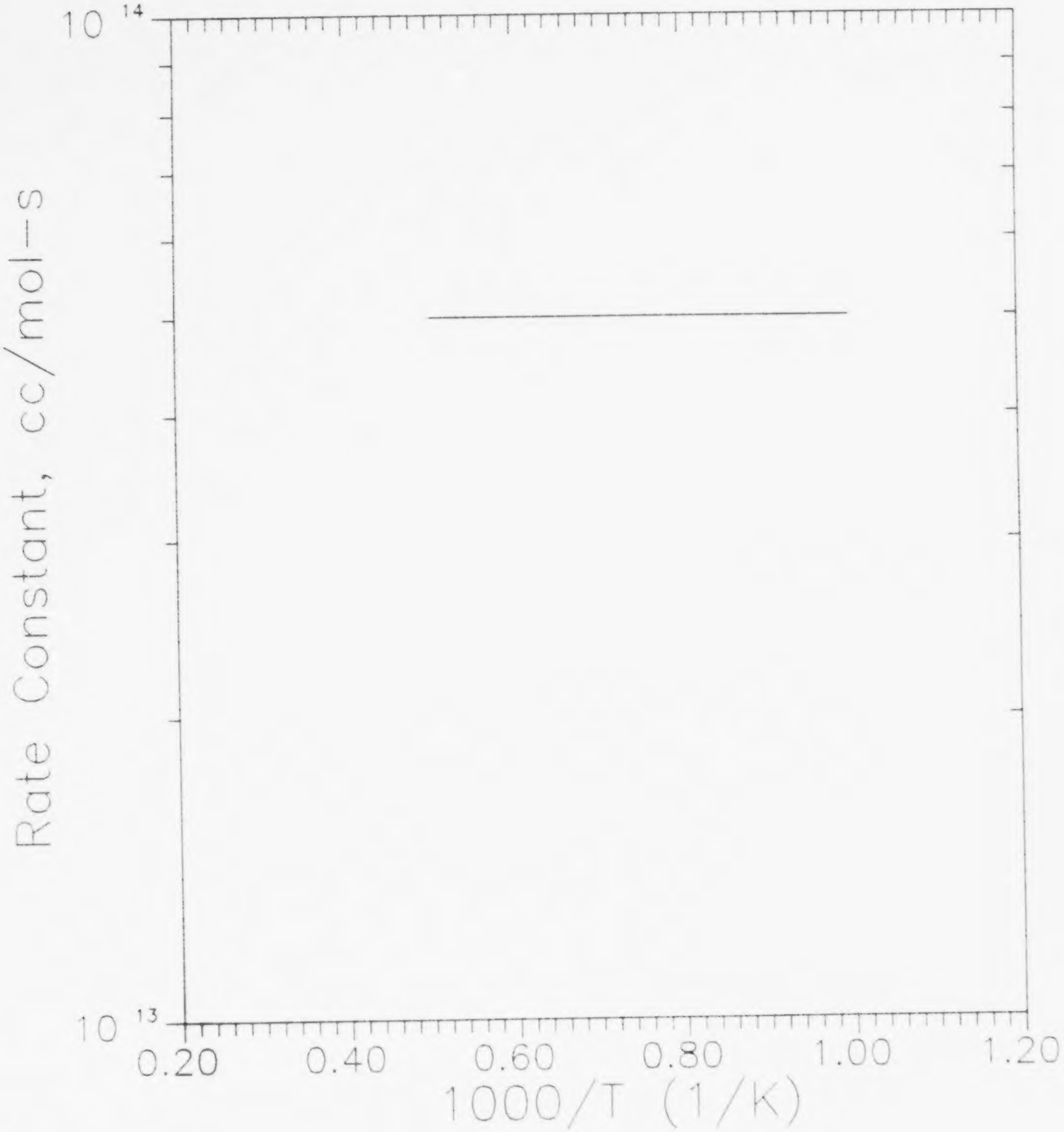
**CH2 + C = C2H + H**



**CH + C2H2 = C2H3 + H**



**CH + C2H2 = CH2 + C2H**


10 ^14
10 ^13
Rate Constant, cc/mol-s
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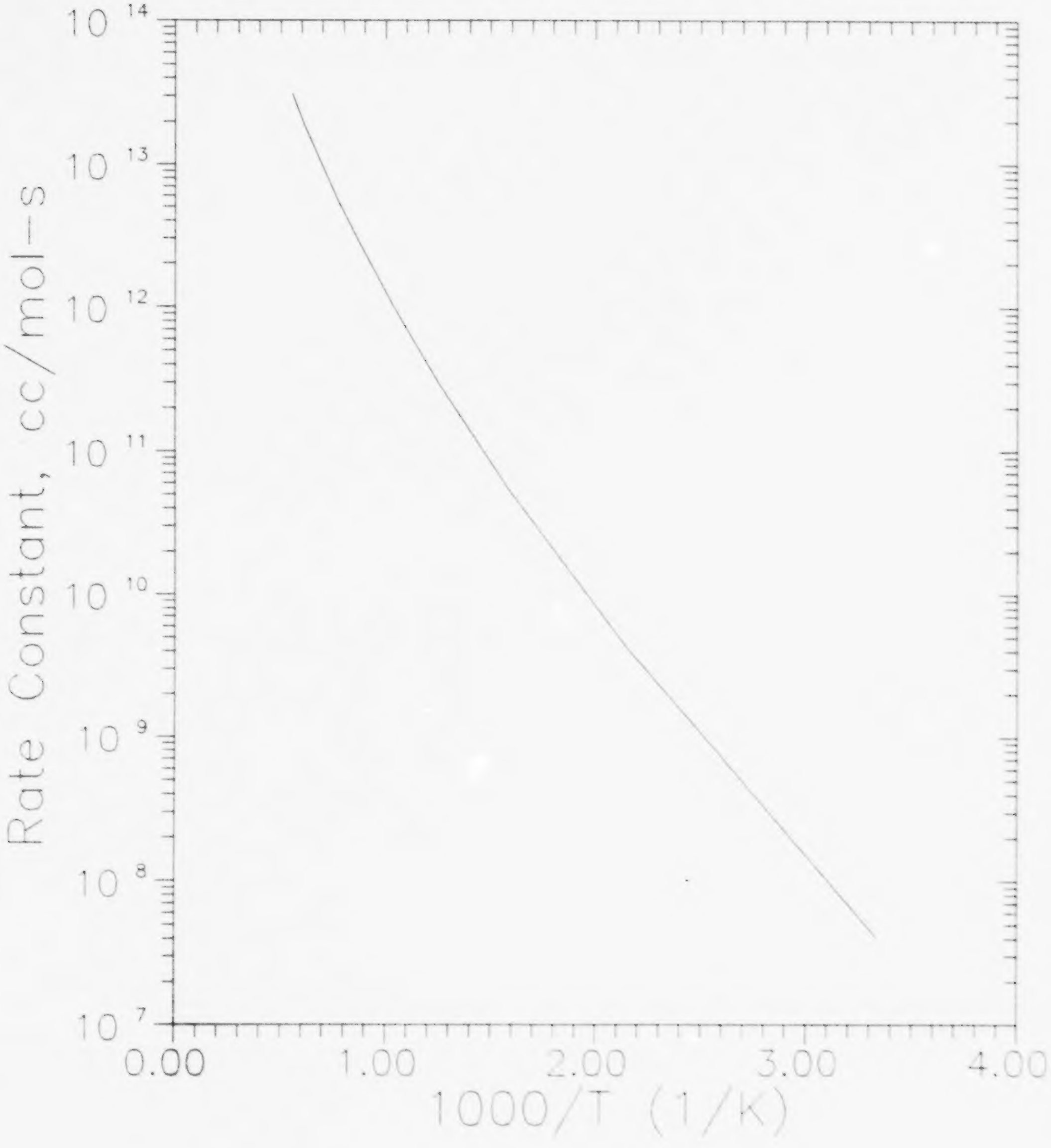
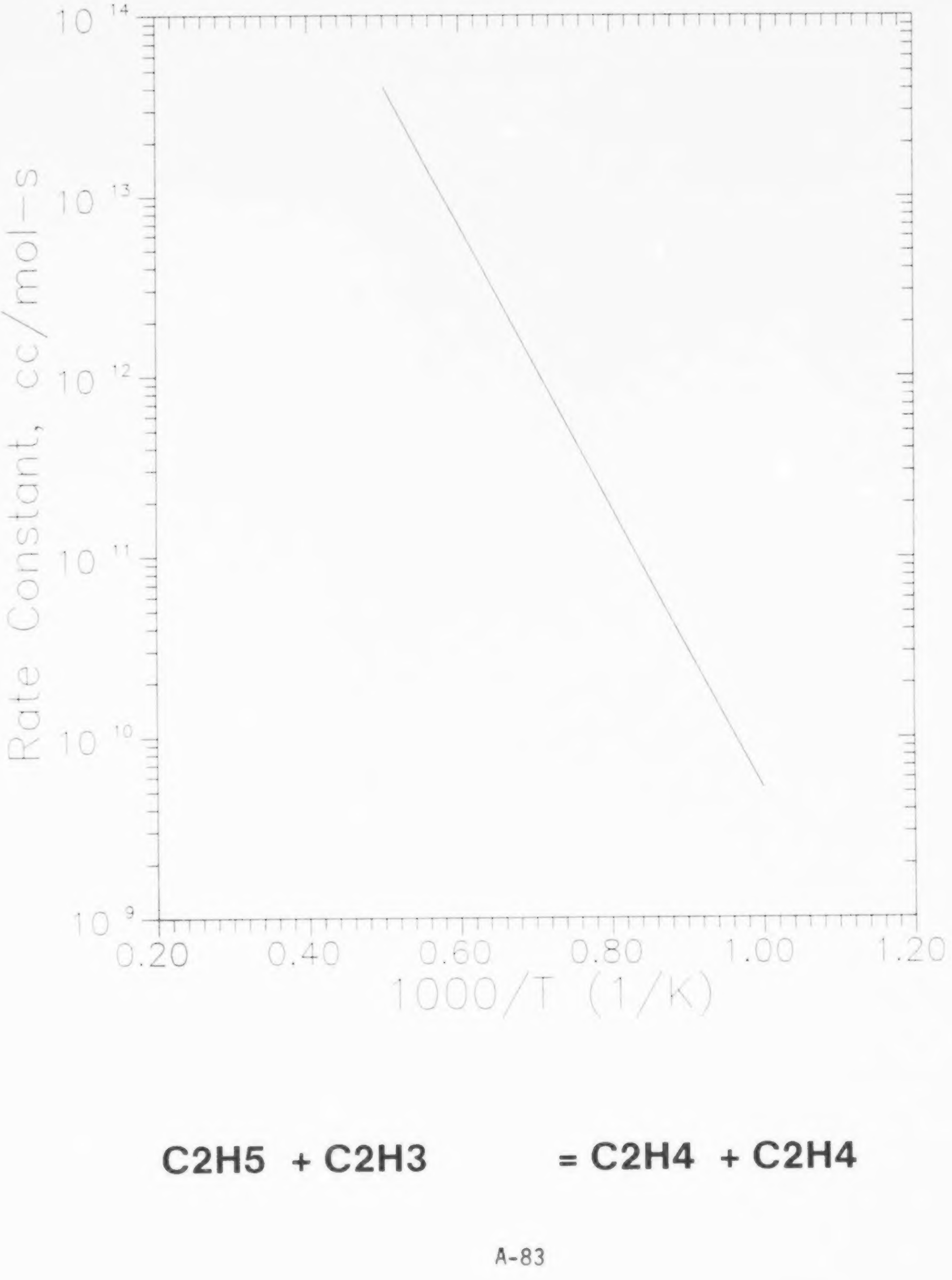
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

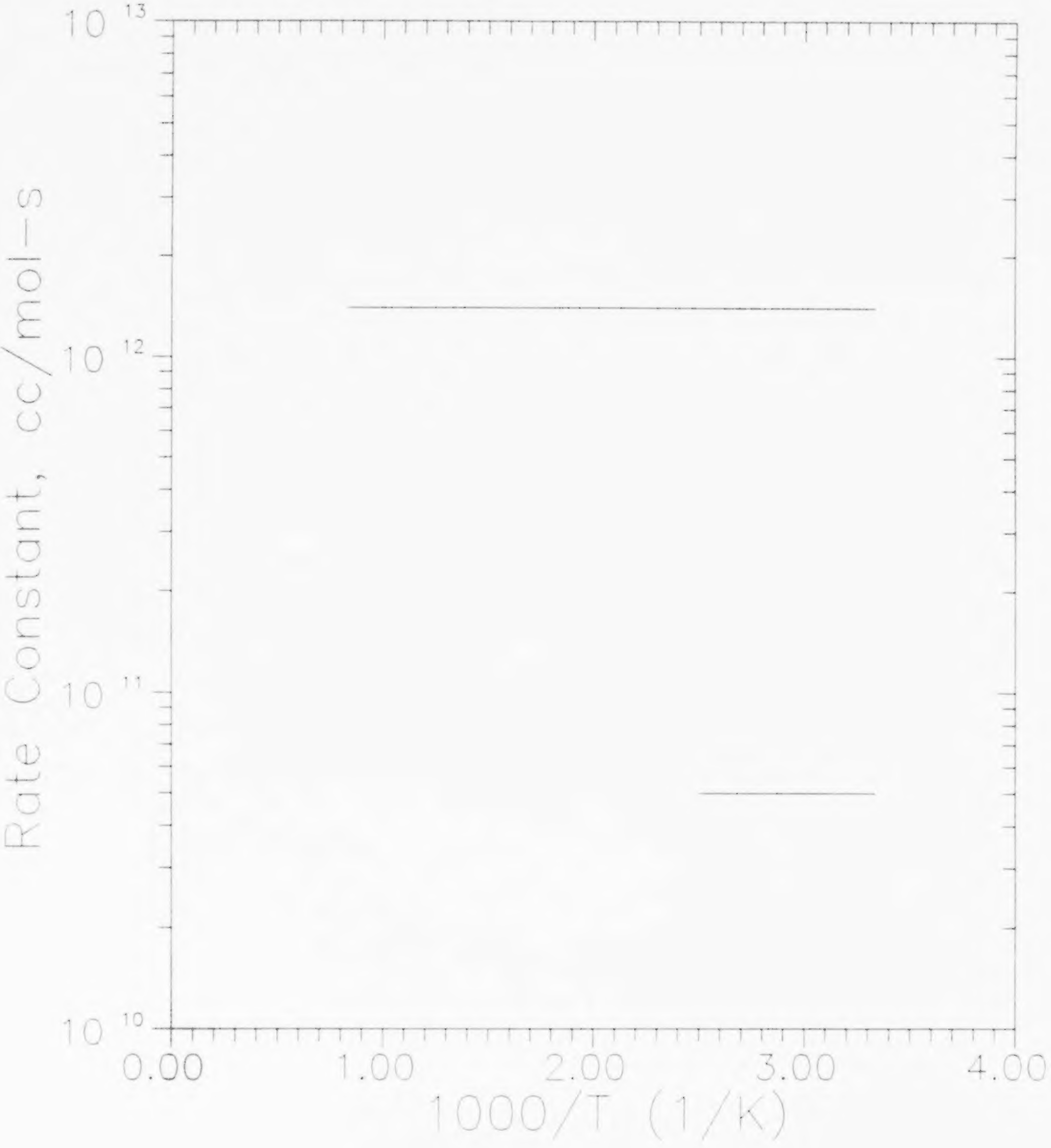
**CH + H = C + H2**



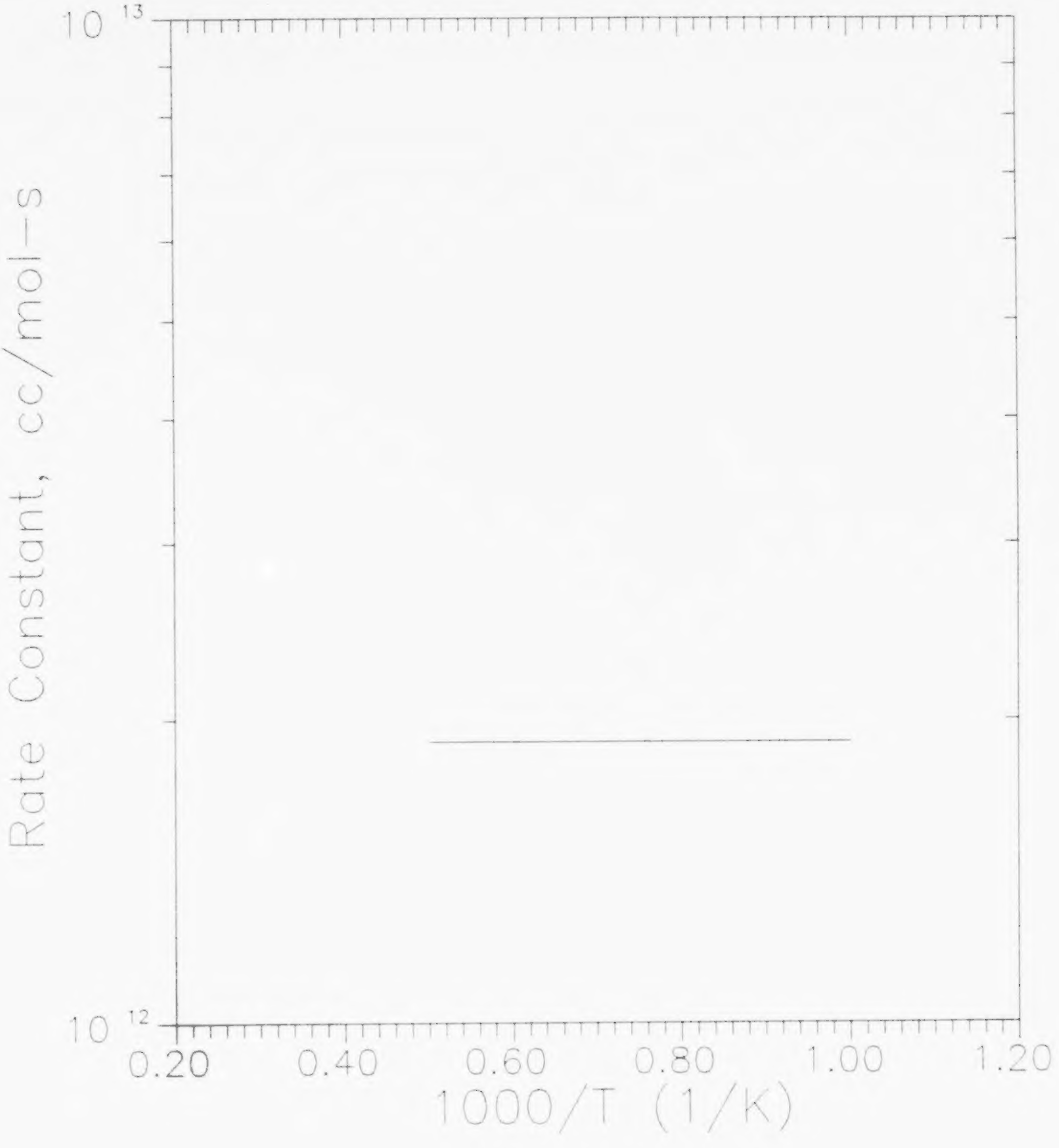
**$C_2H_6 + H = C_2H_5 + H_2$**



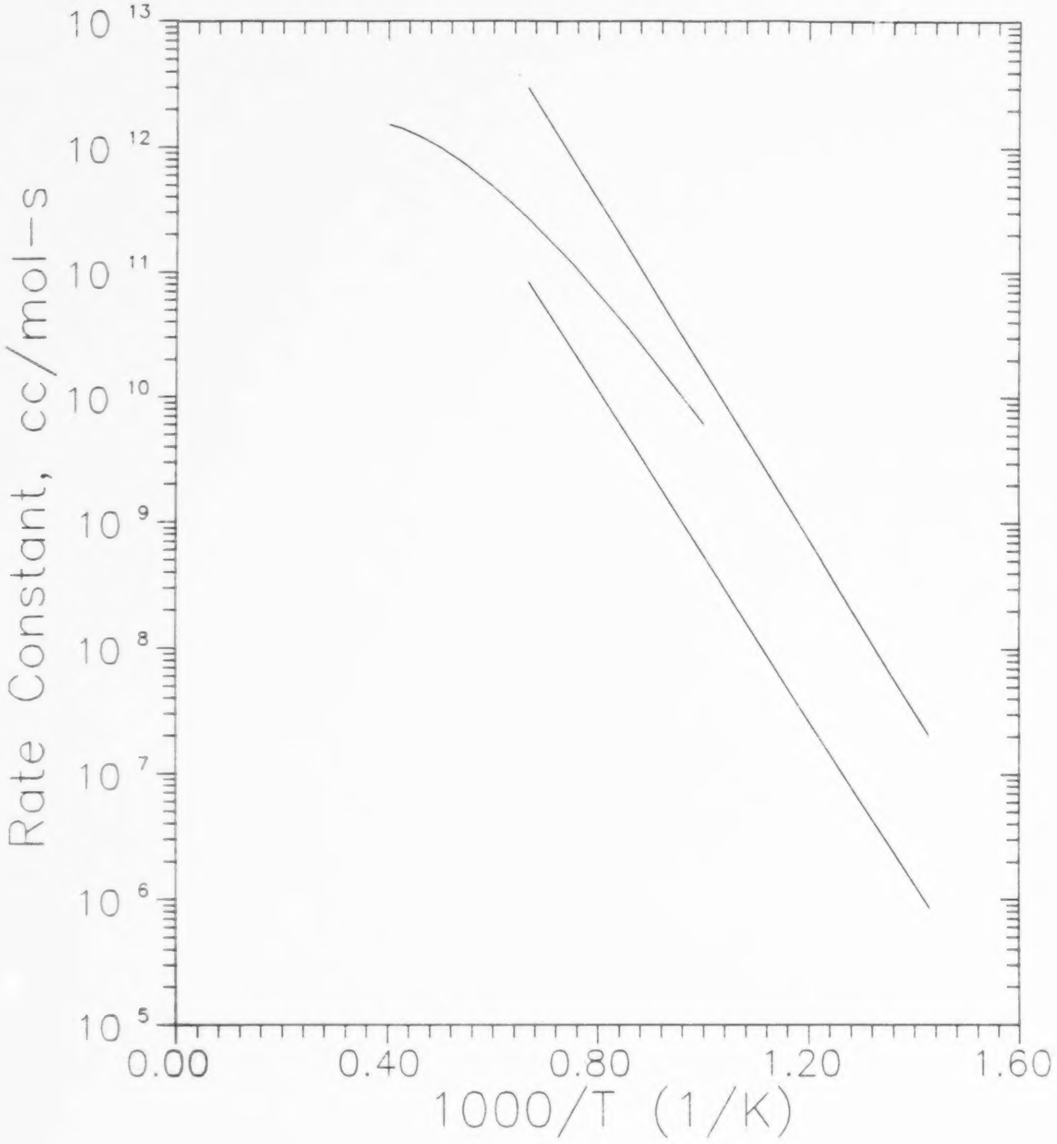
**C2H5 + C2H3 = C2H4 + C2H4**



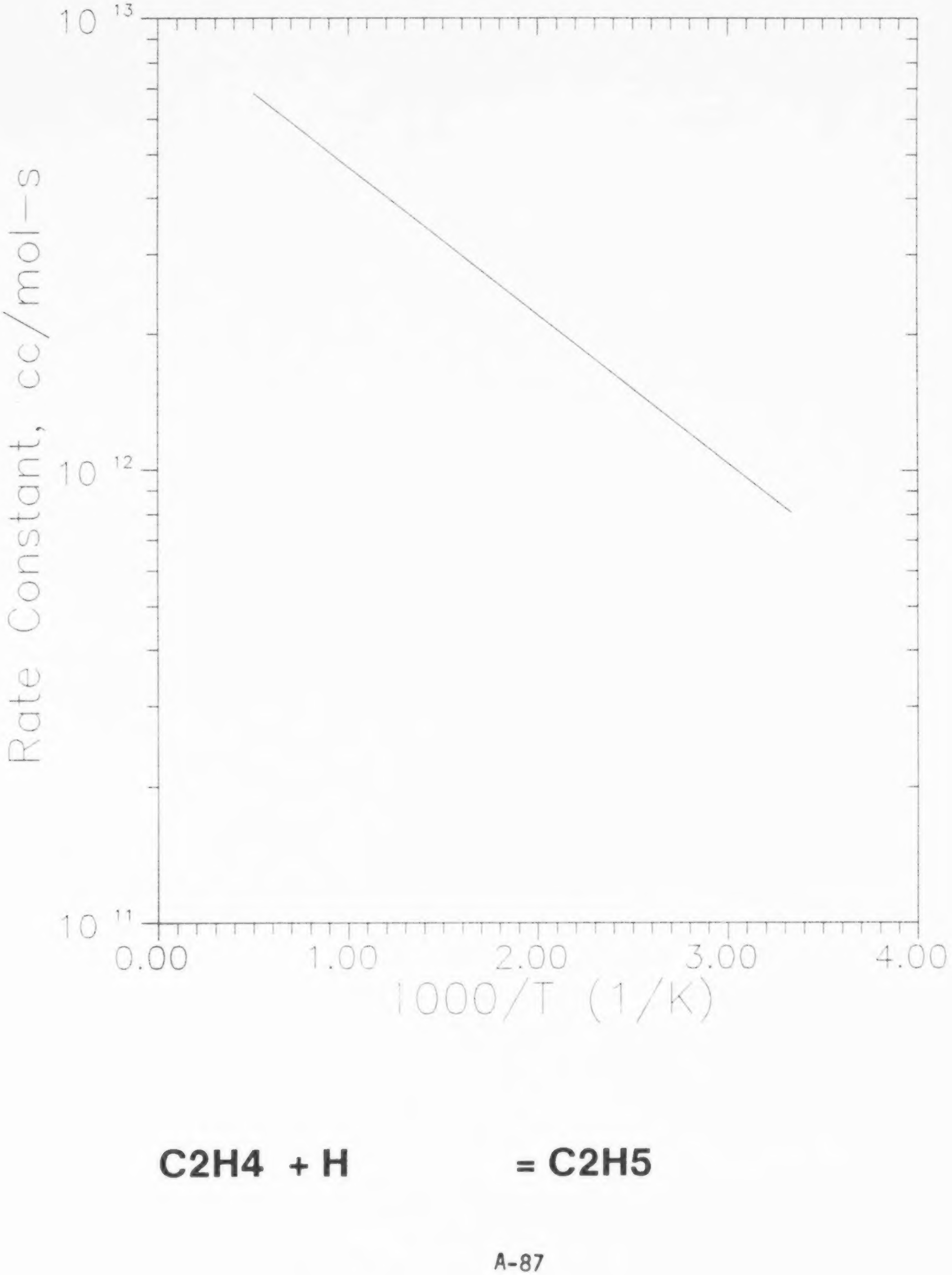
**C2H5 + C2H5 = C2H4 + C2H6**



**C2H5 + H = C2H4 + H2**

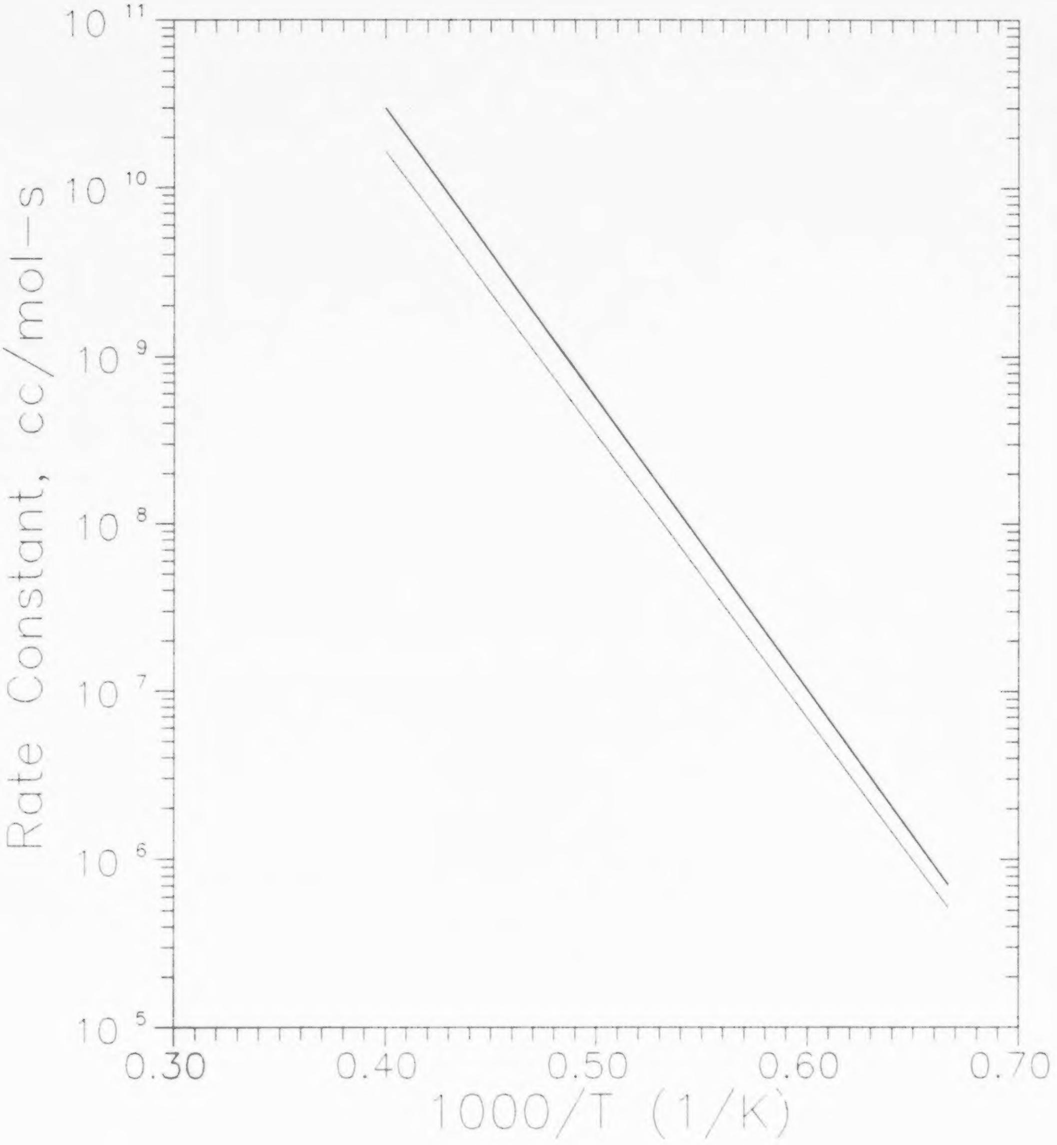


**C2H5 + M = C2H4 + H + M**

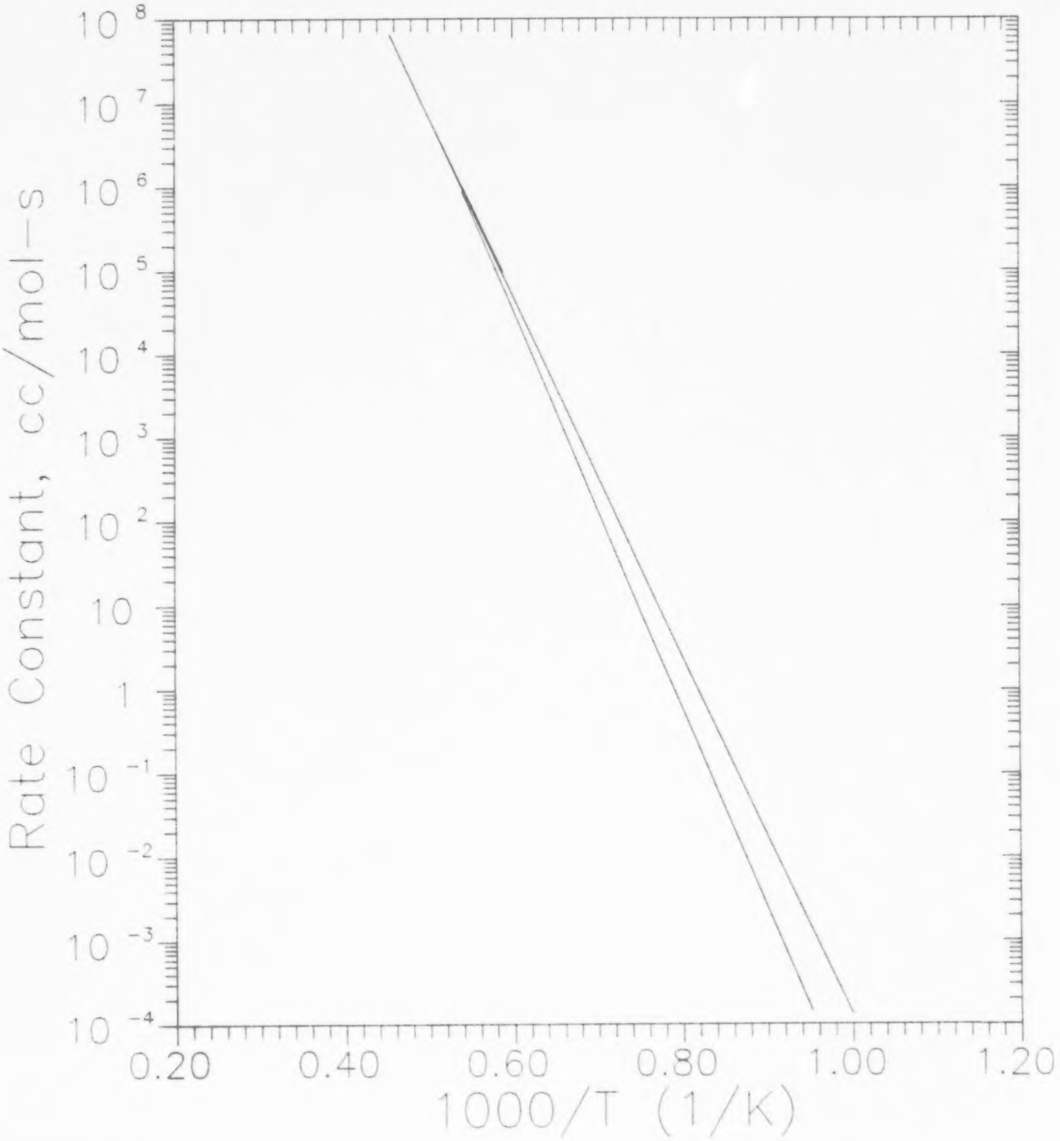


10 13
10 12
10 11
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

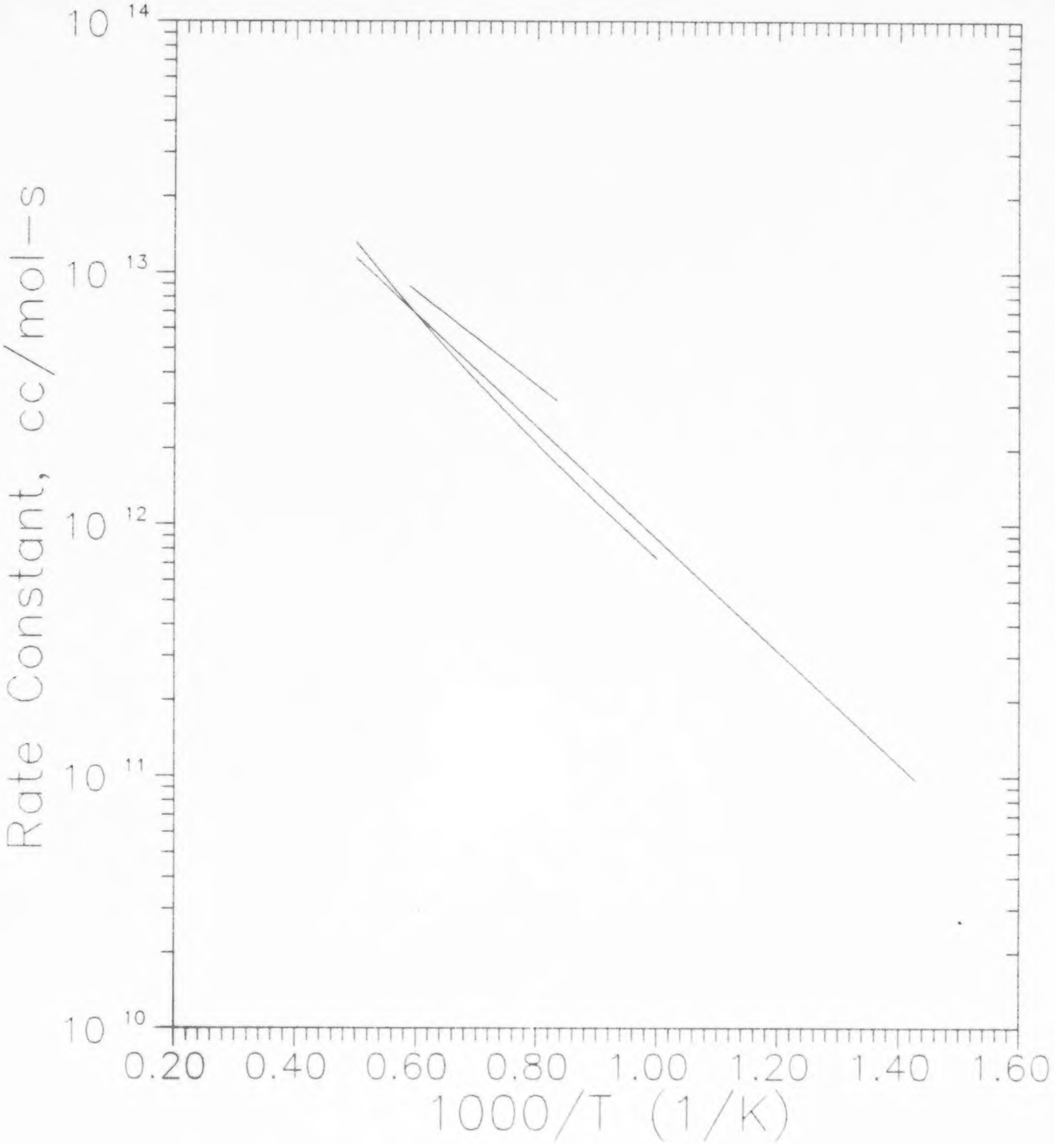
**C2H4 + H = C2H5**



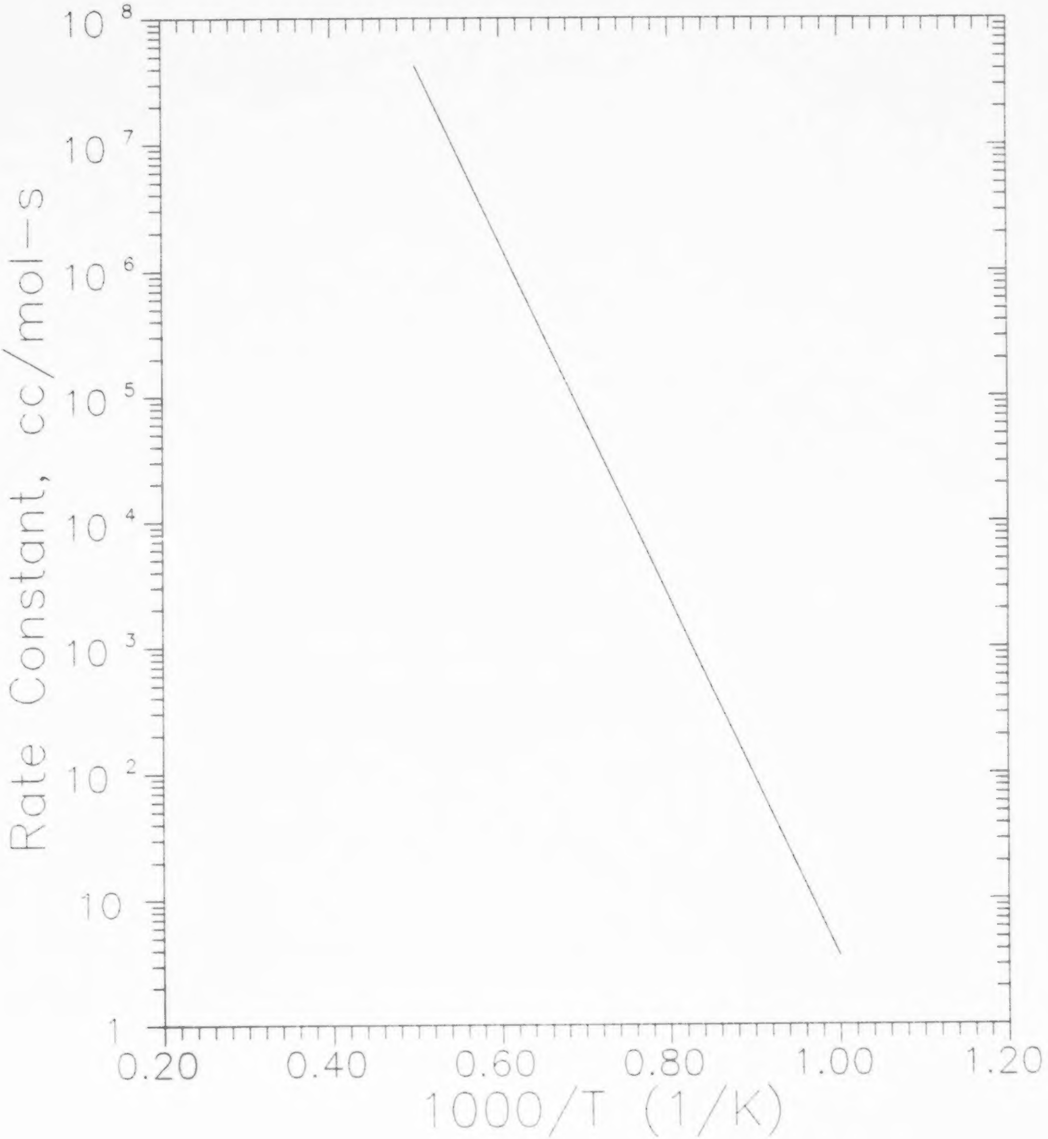
C2H4 + M = C2H2 + H2 + M



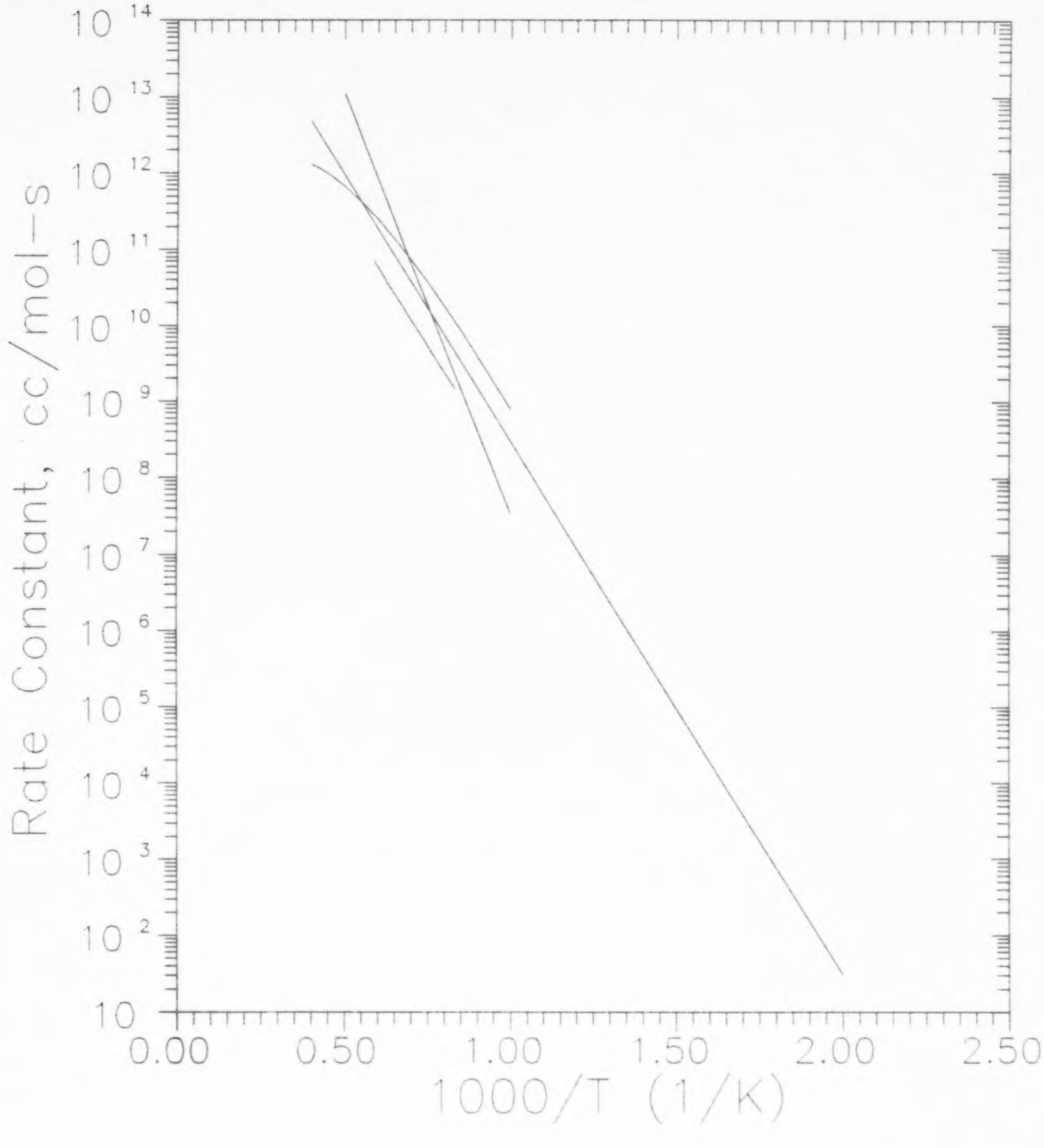
**C2H4 + M = C2H3 + H + M**



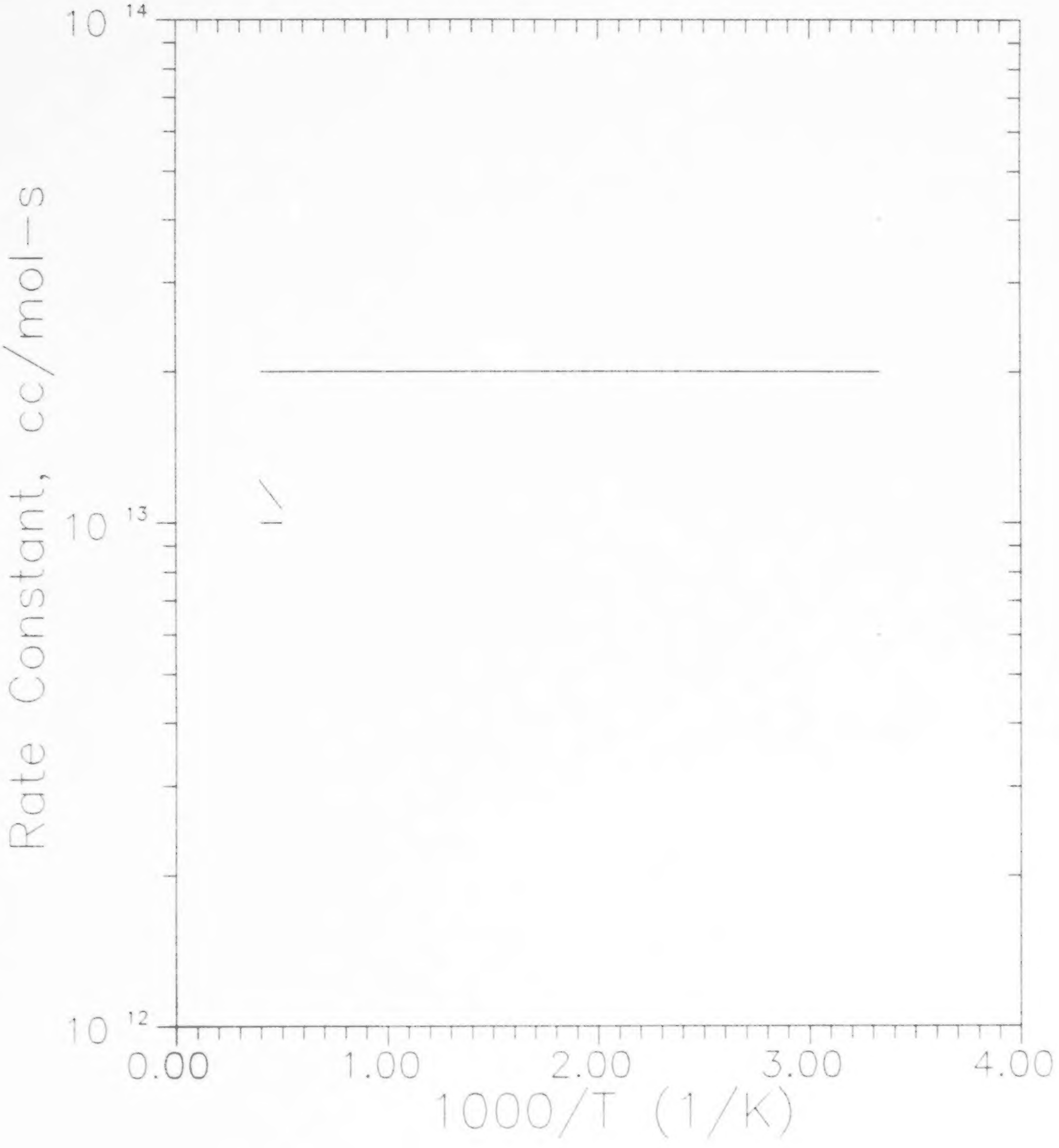
**$C_2H_4$ + H = $C_2H_3$ + $H_2$**



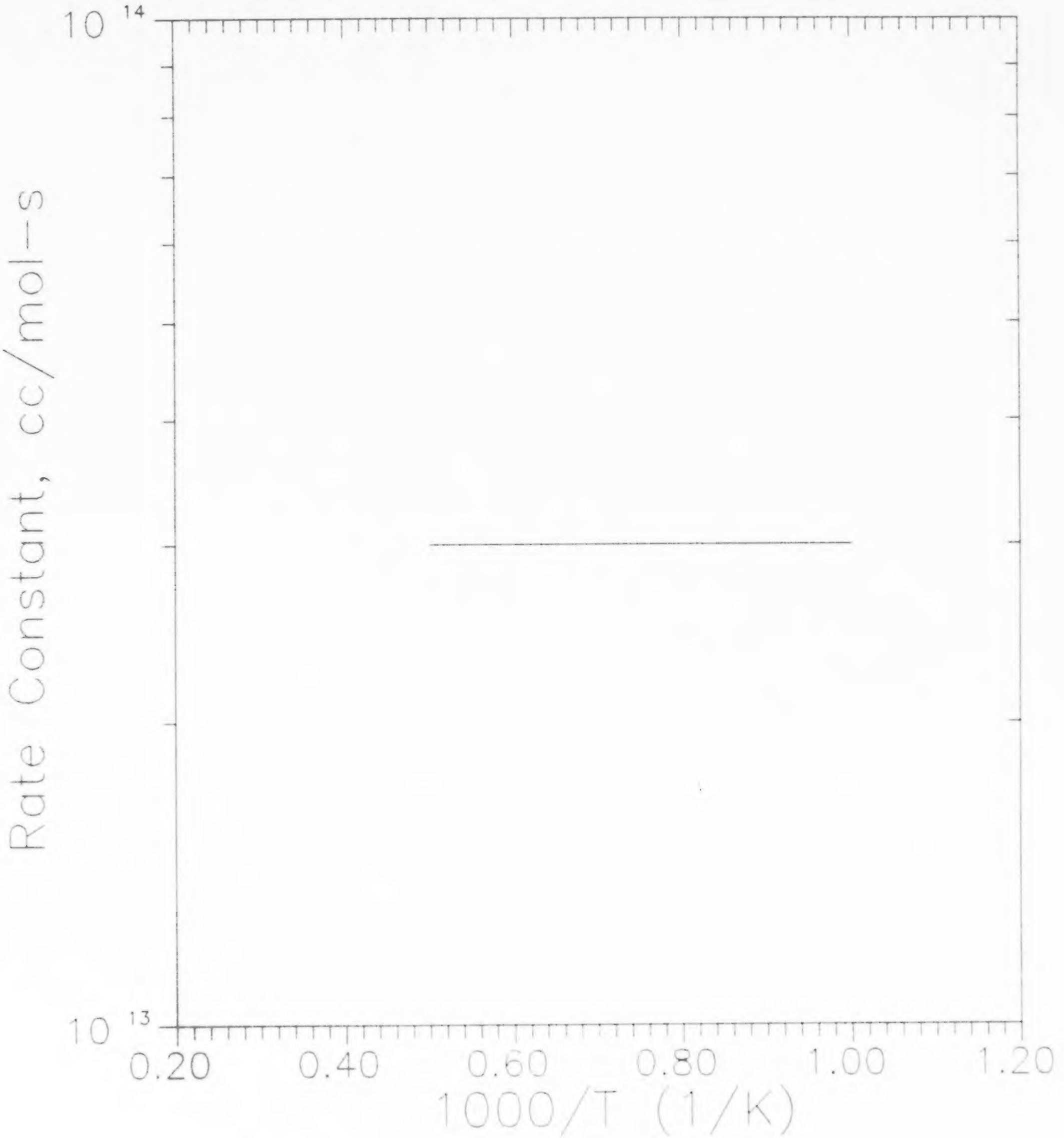
**C2H4 + C2H4 = C2H3 + C2H5**



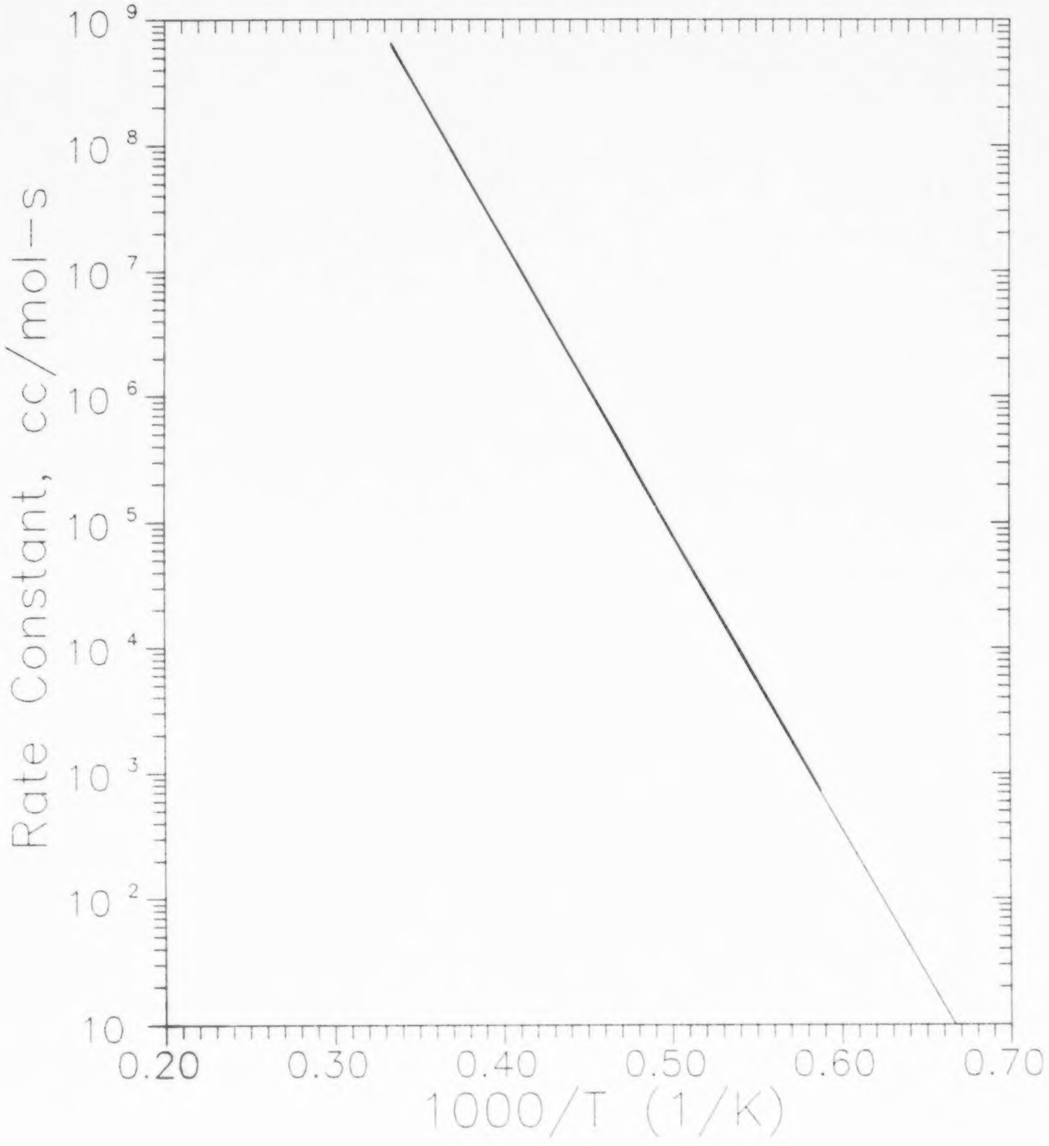
**C2H3 + M = C2H2 + H + M**



**C2H3 + H = C2H2 + H2**

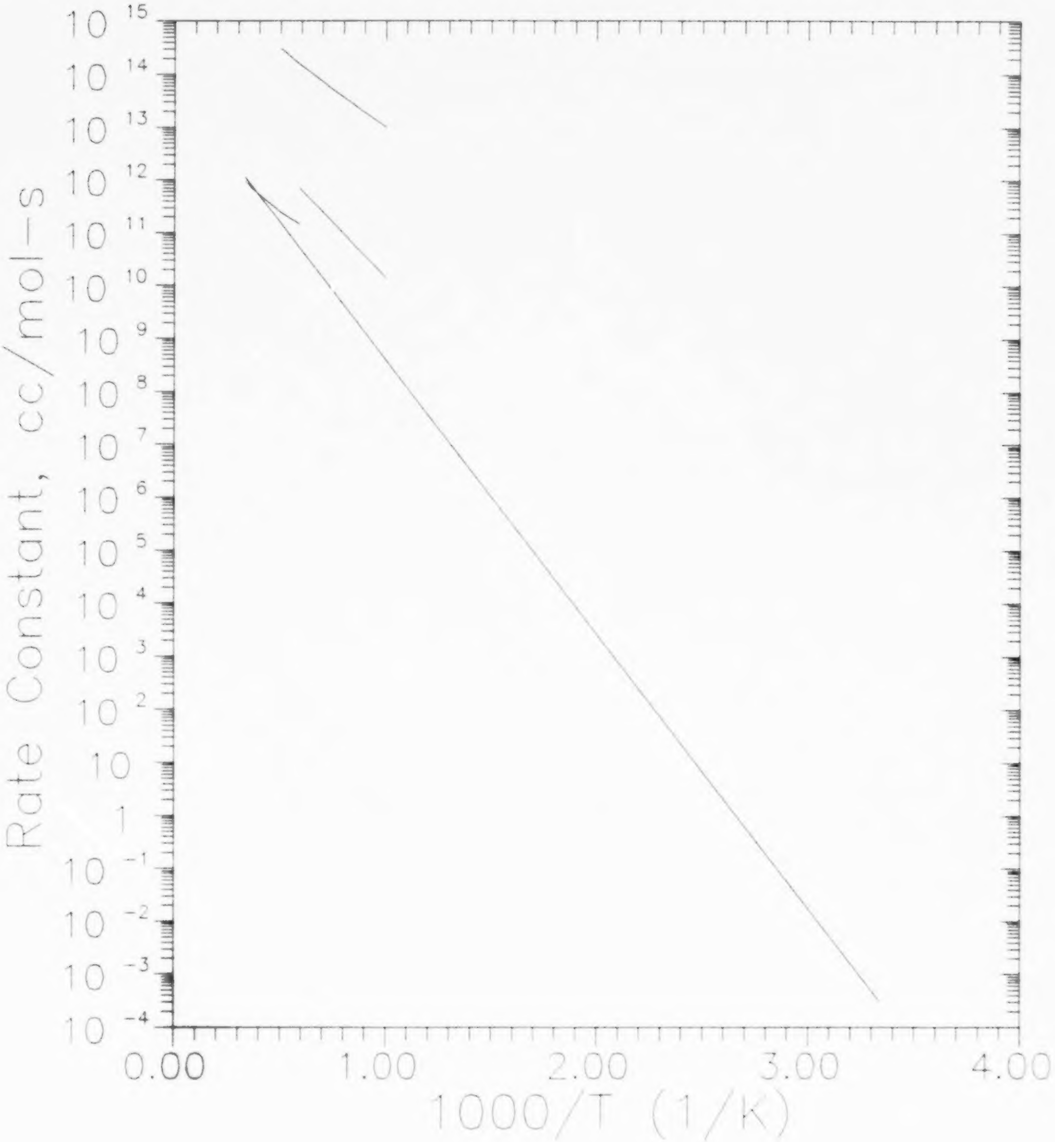


$C2H3 + C2H = C2H2 + C2H2$



Rate Constant, cc/mol-s
10 9
10 8
10 7
10 6
10 5
10 4
10 3
10 2
10
0.20
0.30
0.40
0.50
0.60
0.70
1000/T (1/K)

**C2H2 + M = C2H + H + M**



Rate Constant, cc/mol-s
10 15
10 14
10 13
10 12
10 11
10 10
10 9
10 8
10 7
10 6
10 5
10 4
10 3
10 2
10
1
10 −1
10 −2
10 −3
10 −4
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**$C_2H_2$ + H = $C_2H$ + $H_2$**

```
*---------------------------------------------------------------------------*
|  File: CHOMECH.DAT                                                        |
| Saved: 08-04-88 at 11:03:09 am                                  Page  1  |
*---------------------------------------------------------------------------*

 1CH4  + 1O2            = 1CH3  + 1HO2
Forward Rate Parameters:
Westbrook and Dryer                       7.9E+13 0.000 56.000  1000.0  2000.0
Seeker, et al. 1985                       8.5E+06 2.000 51.970  1000.0  2000.0

 1CH4  + 1HO            = 1CH3  + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                     3.5E+03 3.080  2.000   300.0   900.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985                       1.5E+06 2.100  2.452   300.0  2200.0
Warnatz, Comb. Chem.                      1.6E+06 2.100  2.460   300.0  2200.0

 1CH4  + 1HO2           = 1CH3  + 1H2O2
Forward Rate Parameters:
Seeker, et al. 1985                       2.0E+13 0.000 18.000  1000.0  2000.0
Westbrook and Dryer

 1CH4  + 1O             = 1CH3  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                     1.2E+07 2.080  7.630   300.0  2200.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985
Warnatz, Comb. Chem.

 1CH3  + 1O             = 1CH2O + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                     6.8E+13 0.000  0.000  1500.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                       1.3E+14 0.000  2.000  1150.0  1750.0
Seeker, et al. 1985                       9.0E+13 0.000  2.000  1000.0  2000.0
Warnatz, Comb. Chem.                      7.0E+13 0.000  0.000   300.0  2500.0
Tsang and Hampson. 1986

 1CH3  + 1O             = 1CH2  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                     5.0E+13 0.000 12.000  1000.0  2000.0
Glarborg, et al. 1986
Reverse Rate Parameters:
Seeker, et al. 1985                       5.0E+11 0.500  6.000  1000.0  2000.0

 1CH3  + 1HO            = 1CH2O + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                     4.0E+12 0.000  0.000  1000.0  2000.0
Westbrook and Dryer
Glarborg, et al. 1986                     1.0E+12 0.000  0.000  1000.0  2000.0

 1CH3  + 1HO            = 1CH3O + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                     9.0E+14 0.000 15.400  1000.0  2000.0
Westbrook and Dryer                       2.0E+16 0.000 27.410  1700.0  2300.0
Tsang and Hampson. 1986                   5.4E+13 0.000  0.000   300.0   301.0

 1CH3  + 1HO            = 1CH2  + 1H2O
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*----------------------------------------------------------------------*
|  File: CHOMECH.DAT                                                   |
| Saved: 08-04-88 at 11:03:09 am                             Page  2  |
*----------------------------------------------------------------------*

Forward Rate Parameters:
Glarborg, et al. 1985                  3.0E+13 0.000  3.000  1000.0  2000.0
Glarborg, et al. 1986                  1.5E+13 0.000  5.000  1000.0  2000.0
Seeker, et al. 1985                    6.3E+10 0.700  2.000  1000.0  2000.0

 1CH3  + 102         = 1CH20 + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                  5.2E+13 0.000 34.570  1000.0  2000.0
Glarborg, et al. 1986

 1CH3  + 102         = 1CH30 + 10
Forward Rate Parameters:
Glarborg, et al. 1985                  7.0E+12 0.000 25.650  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                    4.8E+13 0.000 29.000  1000.0  2000.0
Seeker, et al. 1985                    6.0E+09 1.000 28.000  1000.0  2000.0
Warnatz, Comb. Chem.                   1.5E+13 0.000 28.680  1000.0  2300.0

 1CH3  + 1HO2        = 1CH30 + 1HO
Forward Rate Parameters:
Westbrook and Dryer                    2.0E+13 0.000  0.000  1000.0  2000.0

 1CH3  + 1CH20       = 1CHO  + 1CH4
Forward Rate Parameters:
Westbrook and Dryer                    1.0E+10 0.500  6.000  1000.0  2000.0

 1CH3  + 1CHO        = 1CO   + 1CH4
Forward Rate Parameters:
Westbrook and Dryer                    3.0E+11 0.500  0.000  1000.0  2000.0

 1CH2  + 1CHCO       = 1C2H  + 1CH20
Forward Rate Parameters:
Glarborg, et al. 1986                  1.0E+13 0.000  2.000  1000.0  2000.0

 1CH2  + 1CHCO       = 1C2H3 + 1CO
Forward Rate Parameters:
Glarborg, et al. 1986                  3.0E+13 0.000  0.000  1000.0  2000.0

 1CH2  + 102         = 1C02  + 1H    + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                  1.6E+12 0.000  1.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                    3.7E+12 0.000  1.500  1000.0  2000.0

 1CH2  + 102         = 1C02  + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                  6.9E+11 0.000  0.500  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                    1.6E+12 0.000  1.000  1000.0  2000.0

 1CH2  + 102         = 1CO   + 1H20
Forward Rate Parameters:
Glarborg, et al. 1985                  1.9E+10 0.000 -1.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                    1.0E+11 0.000  0.000  1000.0  2000.0
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*------------------------------------------------------------------------------*
| File: CHOMECH.DAT                                                            |
| Saved: 08-04-88 at 11:03:09 am                                       Page  3 |
*------------------------------------------------------------------------------*

Hwang, et al. 1987                        3.9E+12 0.000  1.400  1300.0  2200.0

 1CH2  + 102          = 1CO   + 1HO    + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                     8.6E+10 0.000 -0.500  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                       2.0E+11 0.000  0.000  1000.0  2000.0
Hwang, et al. 1987                        9.1E+12 0.000  1.400  1300.0  2200.0

 1CH2  + 102          = 1CHO  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                     4.3E+10 0.000 -0.500  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                       1.0E+14 0.000  3.700  1200.0  1600.0

 1CH2  + 102          = 1CH2O + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                     5.0E+13 0.000  9.000  1000.0  2000.0
Glarborg, et al. 1986                     2.0E+13 0.000  9.000  1000.0  2000.0
Seeker, et al. 1985                       7.7E+09 1.000  0.540  1000.0  2000.0

 1CH2  + 1O           = 1CO   + 1H     + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                     3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                       5.0E+12 0.000  0.000  1000.0  2000.0

 1CH2  + 1O           = 1CO   + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                     5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                       5.0E+12 0.000  0.000  1000.0  2000.0

 1CH2  + 1O           = 1CH   + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                     5.0E+13 0.000 12.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                       2.0E+11 0.680 25.000  1000.0  2000.0

 1CH2  + 1O           = 1CHO  + 1H
Forward Rate Parameters:
Seeker, et al. 1985                       6.5E+13 0.000  0.000  1000.0  2000.0

 1CH2  + 1HO          = 1CH2O + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                     2.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986                     3.0E+13 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985                       1.0E+13 0.000  5.000  1000.0  2000.0

 1CH2  + 1HO          = 1CH   + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                     3.0E+13 0.000  3.000  1000.0  2000.0
Glarborg, et al. 1986                     4.5E+13 0.000  3.000  1000.0  2000.0
Westbrook and Dryer                       2.5E+11 0.670 25.700  1000.0  2000.0
Seeker, et al. 1985                       5.0E+11 0.500  6.000  1000.0  2000.0
```

```
 1CH2  + 1CO2          = 1CO   + 1CH2O
Forward Rate Parameters:
Glarborg, et al. 1985                      1.1E+11 0.000  1.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH   + 1O            = 1CO   + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                      5.7E+13 0.000  0.000   300.0   301.0
Glarborg, et al. 1986
Seeker, et al. 1985                        5.0E+11 0.500  0.000  1000.0  2000.0
Warnatz, Comb. Chem.                       4.0E+13 0.000  0.000   300.0  2000.0

 1CH   + 1HO           = 1CHO  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                      3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                        5.0E+11 0.500  5.620  1000.0  2000.0

 1CH   + 1O2           = 1CHO  + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                      3.3E+13 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985                        2.0E+13 0.000  0.000   300.0  2000.0
Warnatz, Comb. Chem.
Westbrook and Dryer                        1.0E+13 0.000  0.000  1800.0  2360.0

 1CH   + 1O2           = 1CO   + 1HO
Forward Rate Parameters:
Westbrook and Dryer                        1.3E+11 0.670 25.700  2000.0  2400.0
J. Warnatz, et al., 19th Symposium         2.0E+13 0.000  0.000   300.0  2000.0

 1CH   + 1CO2          = 1CHO  + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985                      3.4E+12 0.000  0.690   297.0   676.0
Glarborg, et al. 1986
Seeker, et al. 1985                        1.0E+10 0.500  6.000  1000.0  2000.0

 1C2H6 + 1O            = 1C2H5 + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                      2.5E+13 0.000  6.360   300.0  1000.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985
Warnatz, Comb. Chem.                       3.0E+07 2.000  5.120   300.0  1500.0

 1C2H6 + 1HO           = 1C2H5 + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                      8.7E+09 1.050  1.810  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985                        6.3E+11 0.000  2.450  1000.0  2000.0
Warnatz, Comb. Chem.                       6.3E+06 2.000  0.645   300.0  2000.0

 1C2H6 + 1O2           = 1C2H5 + 1HO2
Forward Rate Parameters:
```

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Westbrook and Dryer                      1.0E+13 0.000 51.000  1000.0  2000.0

 1C2H5 + 102          = 1C2H4 + 1HO2
Forward Rate Parameters:
Glarborg, et al. 1985                    3.2E+12 0.000  5.020  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                      1.0E+12 0.000  5.000   800.0  1300.0
Westbrook and Dryer
Warnatz, Comb. Chem.                     2.0E+12 0.000  5.000   700.0  2000.0

 1C2H5 + 1O           = 1CH2O + 1CH3
Forward Rate Parameters:
Westbrook and Dryer                      1.0E+13 0.000  0.000  1000.0  2000.0
Warnatz, Comb. Chem.                     5.0E+13 0.000  0.000  1000.0  2000.0

 1C2H4 + 1HO          = 1C2H3 + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                    4.8E+12 0.000  1.230   300.0  1300.0
Glarborg, et al. 1986                    6.3E+12 0.000  1.230   300.0  1300.0
Westbrook and Dryer
Seeker, et al. 1985                      1.0E+14 0.000  3.500   810.0   811.0
Warnatz, Comb. Chem.                     3.0E+13 0.000  3.000   500.0  2000.0

 1C2H4 + 1HO          = 1CH2O + 1CH3
Forward Rate Parameters:
Glarborg, et al. 1985                    2.0E+12 0.000  0.960   810.0  1300.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985                      4.5E+12 0.000  0.220  1000.0  2000.0
Warnatz, Comb. Chem.                     3.0E+13 0.000  3.000   500.0  2000.0

 1C2H4 + 1O           = 1CHO  + 1CH3
Forward Rate Parameters:
Glarborg, et al. 1985                    1.6E+09 1.200  0.746   300.0  2000.0
Glarborg, et al. 1986
Warnatz, Comb. Chem.
Seeker, et al. 1985                      5.9E+10 0.740  0.560   195.0   715.0
Westbrook and Dryer                      3.3E+12 0.000  1.130   810.0  1300.0

 1C2H4 + 1O           = 1CH2O + 1CH2
Forward Rate Parameters:
Seeker, et al. 1985                      8.0E+06 2.000  0.307   300.0   700.0
Westbrook and Dryer                      2.5E+13 0.000  5.000   300.0  1000.0

 1C2H3 + 102          = 1CHO  + 1CH2O
Forward Rate Parameters:
Glarborg, et al. 1985                    4.0E+12 0.000 -0.250  1000.0  2000.0
Glarborg, et al. 1986

 1C2H3 + 102          = 1C2H2 + 1HO2
Forward Rate Parameters:
Westbrook and Dryer                      1.0E+12 0.000 10.000  1058.0  1876.0
Warnatz, Comb. Chem.                     1.0E+12 0.000  0.000  1000.0  2000.0

 1C2H3 + 1O           = 1CH2CO+ 1H
```

```
Forward Rate Parameters:
Glarborg, et al. 1985                   3.3E+13 0.000  0.000   300.0   301.0
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, Comb. Chem.                    3.0E+13 0.000  0.000   300.0  2000.0

 1C2H3 + 1HO          = 1C2H2 + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                   5.0E+12 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer

 1C2H2 + 1O2          = 1CHO  + 1CHO
Forward Rate Parameters:
Seeker, et al. 1985                     4.0E+12 0.000 28.000  1000.0  2000.0
Westbrook and Dryer

 1C2H2 + 1O           = 1CH2  + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985                   2.2E+10 1.000  2.580   300.0  2500.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985                     6.7E+13 0.000  4.000   700.0  1430.0
Warnatz, Comb. Chem.                    4.1E+08 1.500  1.700   300.0  2500.0

 1C2H2 + 1O           = 1C2H  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                   3.2E+15-0.600 15.000  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985                     3.2E+15-0.600 17.000  1000.0  2000.0

 1C2H2 + 1O           = 1CHCO + 1H
Forward Rate Parameters:
Glarborg, et al. 1986                   3.6E+04 2.700  1.390   300.0  2500.0
Westbrook and Dryer
Warnatz, Comb. Chem.                    4.3E+14 0.000 12.120  1000.0  2500.0

 1C2H2 + 1HO          = 1CH2CO+ 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   3.2E+11 0.000  0.200  1000.0  2000.0
Glarborg, et al. 1986

 1C2H2 + 1HO          = 1CH3  + 1CO
Forward Rate Parameters:
Seeker, et al. 1985                     5.5E+13 0.000 13.700  1000.0  2000.0
Westbrook and Dryer                     1.2E+12 0.000  0.500   300.0   460.0

 1C2H2 + 1HO          = 1C2H  + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                   6.0E+12 0.000  7.000  1000.0  1700.0
Glarborg, et al. 1986                   6.3E+12 0.000  7.000  1000.0  1700.0
Westbrook and Dryer
Seeker, et al. 1985                     1.4E+13 0.000  7.000  1000.0  2000.0
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 1C2H  + 10            = 1CH   + 1CO
Forward Rate Parameters:
Glarborg, et al. 1986                     5.0E+13 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985
Westbrook and Dryer

 1C2H  + 102           = 1CHCO + 10
Forward Rate Parameters:
Glarborg, et al. 1986                     6.0E+11 0.000  0.000   300.0  1000.0
Westbrook and Dryer                       3.3E+12 0.000  0.000   320.0   321.0
Warnatz, Comb. Chem.                      5.0E+13 0.000  1.510   300.0  2500.0

 1C2H  + 102           = 1CHO  + 1CO
Forward Rate Parameters:
Glarborg, et al. 1986                     2.4E+12 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985                       1.0E+13 0.000  7.000  1000.0  2000.0
Westbrook and Dryer

 1C2H  + 1HO           = 1CHCO + 1H
Forward Rate Parameters:
Glarborg, et al. 1986                     2.0E+13 0.000  0.000  1000.0  2000.0

 1C2H  + 1HO           = 1CH2  + 1CO
Forward Rate Parameters:
Seeker, et al. 1985                       6.0E+12 0.000  0.000  1000.0  2000.0

 1CH3O + 1M            = 1CH2O + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                     1.0E+14 0.000 25.000  1000.0  2200.0
Glarborg, et al. 1986
Seeker, et al. 1985
Warnatz, Comb. Chem.
Westbrook and Dryer                       5.0E+13 0.000 21.000  1200.0  1800.0

 1CH3O + 10            = 1CH2O + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                     1.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                       1.0E+14 0.000  0.000  1000.0  2000.0

 1CH3O + 102           = 1CH2O + 1HO2
Forward Rate Parameters:
Glarborg, et al. 1985                     6.3E+10 0.000  2.600  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                       1.0E+12 0.000  6.000  1000.0  2000.0
Warnatz, Comb. Chem.                      1.0E+13 0.000  7.200   300.0  2000.0

 1CH3O + 1H            = 1CH2O + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                     2.0E+13 0.000  0.000   300.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, Comb. Chem.
Seeker, et al. 1985                       1.0E+14 0.000  0.000  1000.0  2000.0
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 1CH3O + 1HO           = 1CH2O + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                   1.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                     3.0E+13 0.000  0.000  1000.0  2000.0

 1CH2O + 1M            = 1CHO  + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                   3.3E+16 0.000 81.000  1600.0  3000.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985
Warnatz, Comb. Chem.                    5.0E+16 0.000 76.500  1000.0  3000.0

 1CH2O + 1O            = 1CHO  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                   1.8E+13 0.000  3.080  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer                     5.0E+13 0.000  4.600  1875.0  2240.0
Warnatz, Comb. Chem.                    3.5E+13 0.000  3.510   300.0  2500.0
Seeker, et al. 1985                     1.3E+10 1.000  2.050  1000.0  2000.0

 1CH2O + 1H            = 1CHO  + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                   3.3E+14 0.000 10.500  1600.0  3000.0
Westbrook and Dryer
Glarborg, et al. 1986                   2.2E+08 1.770 10.500  1000.0  2000.0
Seeker, et al. 1985                     2.5E+10 1.000  3.200  1000.0  2000.0
Warnatz, Comb. Chem.                    2.5E+13 0.000  4.000   300.0  2500.0

 1CH2O + 1HO           = 1CHO  + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                   7.5E+12 0.000  0.170   300.0   420.0
Westbrook and Dryer
Glarborg, et al. 1986                   3.4E+09 1.180 -0.440   300.0  1000.0
Seeker, et al. 1985                     5.0E+09 1.000  1.650  1000.0  2000.0
Warnatz, Comb. Chem.                    3.0E+13 0.000  1.200   300.0  2500.0

 1CH2O + 1HO2          = 1CHO  + 1H2O2
Forward Rate Parameters:
Seeker, et al. 1985                     1.0E+12 0.000  8.000  1000.0  2000.0
Westbrook and Dryer

 1CHO  + 1M    +       = 1CO   + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                   1.6E+14 0.000 14.700  1400.0  2200.0
Glarborg, et al. 1986                   1.5E+14 0.000 14.675  1000.0  2000.0
Seeker, et al. 1985
Westbrook and Dryer                     1.4E+14 0.000 19.000  1000.0  1350.0
Warnatz, Comb. Chem.                    2.5E+14 0.000 16.800   700.0  2500.0

 1CHO  + 1O2   +       = 1CO   + 1HO2  +
Forward Rate Parameters:
Glarborg, et al. 1985                   3.3E+13-0.400  0.000   300.0   500.0
Glarborg, et al. 1986
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Westbrook and Dryer                     3.3E+12 0.000  7.000  1000.0  1350.0
Seeker, et al. 1985                     5.0E+11 0.500  0.834  1000.0  2000.0
Warnatz, Comb. Chem.                    3.0E+12 0.000  0.000   300.0  2000.0
Tsang and Hampson. 1986                 5.12E13 0.000  1.690   300.0  1500.0

 1CHO  + 1O    +      = 1CO   + 1HO   +
Forward Rate Parameters:
Glarborg, et al. 1985                   3.0E+13 0.000  0.000   300.0  2000.0
Glarborg, et al. 1986
Warnatz, Comb. Chem.
Westbrook and Dryer                     1.0E+14 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985                     5.5E+12 0.500  0.000  1000.0  2000.0

 1CHO  + 1O    +      = 1CO2  + 1H    +
Forward Rate Parameters:
Glarborg, et al. 1985                   3.0E+13 0.000  0.000   300.0  2000.0
Glarborg, et al. 1986
Warnatz, Comb. Chem.
Seeker, et al. 1985                     5.5E+12 0.500  0.000  1000.0  2000.0

 1CHO  + 1H    +      = 1CO   + 1H2   +

Forward Rate Parameters:
Glarborg, et al. 1985                   4.0E+13 0.000  0.000  1100.0  1101.0
Glarborg, et al. 1986
Seeker, et al. 1985                     2.0E+14 0.000  0.000  1700.0  2710.0
Westbrook and Dryer
Warnatz, Comb. Chem.
Tsang and Hampson. 1986                 1.2E+14 0.000  0.000   300.0   301.0

 1CHO  + 1HO   +      = 1CO   + 1H2O  +
Forward Rate Parameters:
Glarborg, et al. 1985                   1.0E+14 0.000  0.000  1875.0  2240.0
Westbrook and Dryer
Seeker, et al. 1985                     3.0E+10 1.000  0.000  1000.0  2000.0
Warnatz, Comb. Chem.                    5.0E+13 0.000  0.000  1000.0  2500.0
Glarborg, et al. 1986                   5.0E+12 0.000  0.000  1000.0  2000.0
Tsang and Hampson. 1986                 3.0E+13 0.000  0.000  1000.0  2000.0


 1CHO  + 1CHO  +      = 1CO   + 1CH2O +
Forward Rate Parameters:
Seeker, et al. 1985                     4.0E+13 0.000  0.000  1000.0  2000.0

 1CH2CO+ 1M    +      = 1CH2  + 1CO   + 1M
Forward Rate Parameters:
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Glarborg, et al. 1986
Warnatz, Comb. Chem.

 1CH2CO+ 1O    +      = 1CH2O + 1CO   +
Forward Rate Parameters:
Glarborg, et al. 1985                   2.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
```

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 1CH2CO+ 1O     +       = 1CHCO + 1HO    +
Forward Rate Parameters:
Glarborg, et al. 1986                 5.0E+13 0.000  8.000  1000.0  2000.0
Westbrook and Dryer                   1.0E+13 0.000  0.000  1000.0  2000.0

 1CH2CO+ 1H     +       = 1CH3  + 1CO    +
Forward Rate Parameters:
Glarborg, et al. 1985                 1.1E+13 0.000  3.430   300.0   500.0
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, Comb. Chem.                  7.0E+12 0.000  3.010   200.0   500.0

 1CH2CO+ 1H     +       = 1CHCO + 1H2    +
Forward Rate Parameters:
Glarborg, et al. 1986                 7.5E+13 0.000  8.000  1000.0  2000.0
Westbrook and Dryer

 1CH2CO+ 1HO    +       = 1CH2O + 1CHO   +
Forward Rate Parameters:
Glarborg, et al. 1985                 2.8E+13 0.000  0.000   480.0  1000.0
Glarborg, et al. 1986
Westbrook and Dryer
Warnatz, Comb. Chem.                  1.0E+13 0.000  0.000   300.0  1000.0

 1CH2CO+ 1HO    +       = 1CHCO + 1H2O   +
Forward Rate Parameters:
Glarborg, et al. 1986                 7.5E+12 0.000  3.000  1000.0  2000.0
Westbrook and Dryer                   1.0E+13 0.000  0.000  1000.0  2000.0

 1CHCO + 1H     +       = 1CH2  + 1CO    +
Forward Rate Parameters:
Glarborg, et al. 1986                 1.1E+14 0.000  0.000  1000.0  2000.0
Westbrook and Dryer                   5.0E+12 0.000  0.000  1000.0  2000.0
Warnatz, Comb. Chem.                  3.0E+13 0.000  0.000  1000.0  2500.0

 1CHCO + 1O     +       = 1CO   + 1CO    + 1H
Forward Rate Parameters:
Glarborg, et al. 1986                 1.1E+14 0.000  0.000  1000.0  2000.0
Westbrook and Dryer                   1.2E+12 0.000  0.000   300.0   301.0
Warnatz, Comb. Chem.

 1CHCO + 1HO    +       = 1CHO  + 1CO    + 1H
Forward Rate Parameters:
Glarborg, et al. 1986                 1.0E+13 0.000  0.000  1000.0  2000.0
Westbrook and Dryer                   2.0E+12 0.000  0.000  1000.0  2000.0

 1CHCO + 1O2    +       = 1CO   + 1CO    + 1HO
Forward Rate Parameters:
Glarborg, et al. 1986                 1.5E+12 0.000  2.500  1000.0  2000.0
Westbrook and Dryer                   6.3E+11 0.000  2.000  1000.0  2000.0
Warnatz, Comb. Chem.                  2.0E+13 0.000  0.000  1000.0  2000.0

 1CHCO + 1CHCO +        = 1C2H2 + 1CO    + 1CO
Forward Rate Parameters:
Glarborg, et al. 1986                 1.0E+13 0.000  0.000  1000.0  2000.0
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 1CO    + 1HO    +         = 1CO2   + 1H     +
Forward Rate Parameters:
Glarborg, et al. 1985                  1.5E+07 1.300 -0.760  1000.0  2000.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985
Warnatz, Comb. Chem.                   4.4E+06 1.500 -0.740   300.0  2000.0
This work                              5.47E00 3.140 -4.970  1000.0  2500.0

 1CO    + 1HO2   +         = 1CO2   + 1HO    +
Forward Rate Parameters:
Glarborg, et al. 1985                  5.8E+13 0.000 22.930   770.0   771.0
Glarborg, et al. 1986
Westbrook and Dryer
Seeker, et al. 1985                    1.0E+11 0.000 10.000   700.0  1100.0
Warnatz, Comb. Chem.                   1.5E+14 0.000 23.590   700.0  1100.0


 1C     + 1HO    +         = 1CO    + 1H     +
Forward Rate Parameters:
Glarborg, et al. 1985                  5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
```
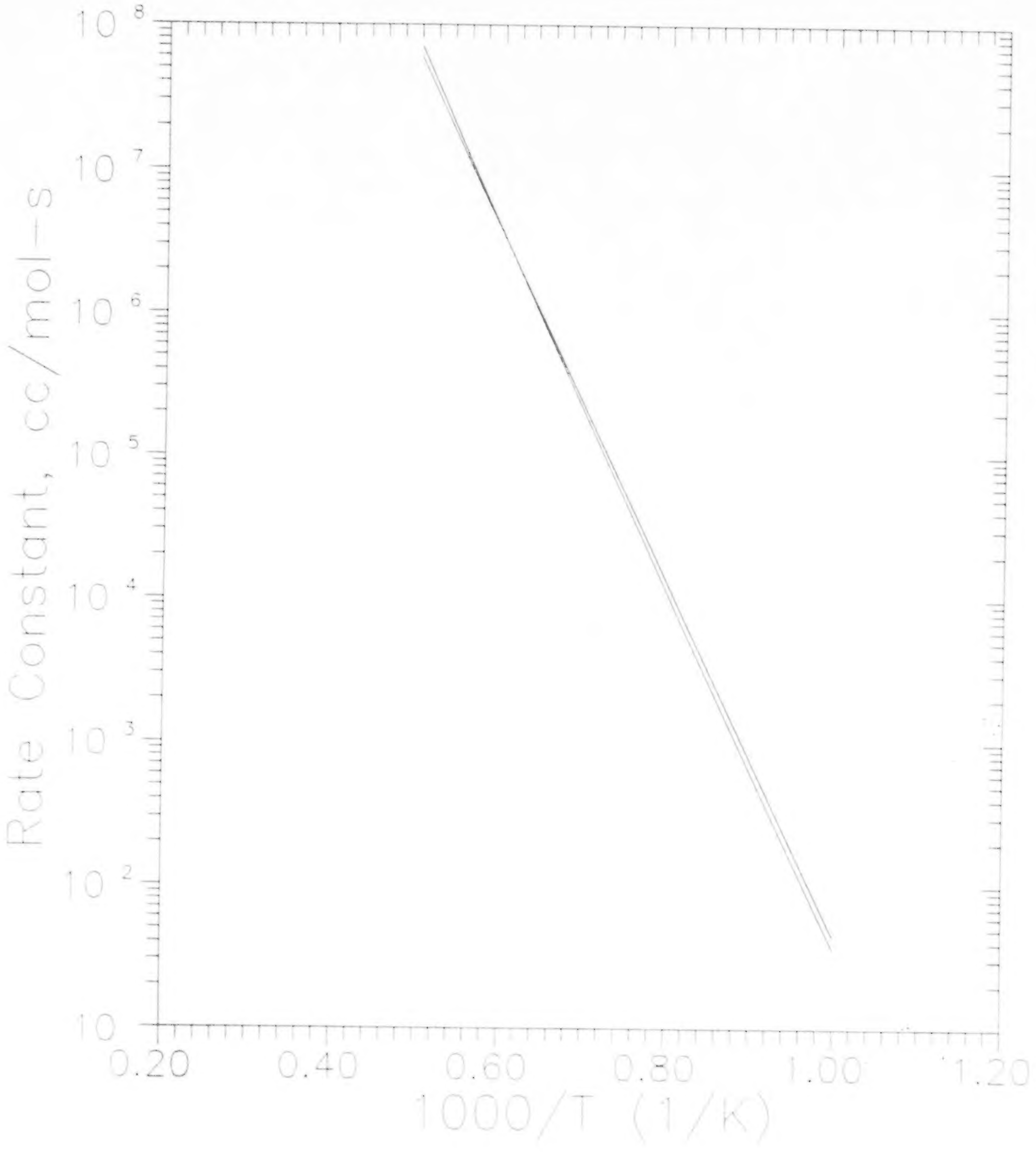
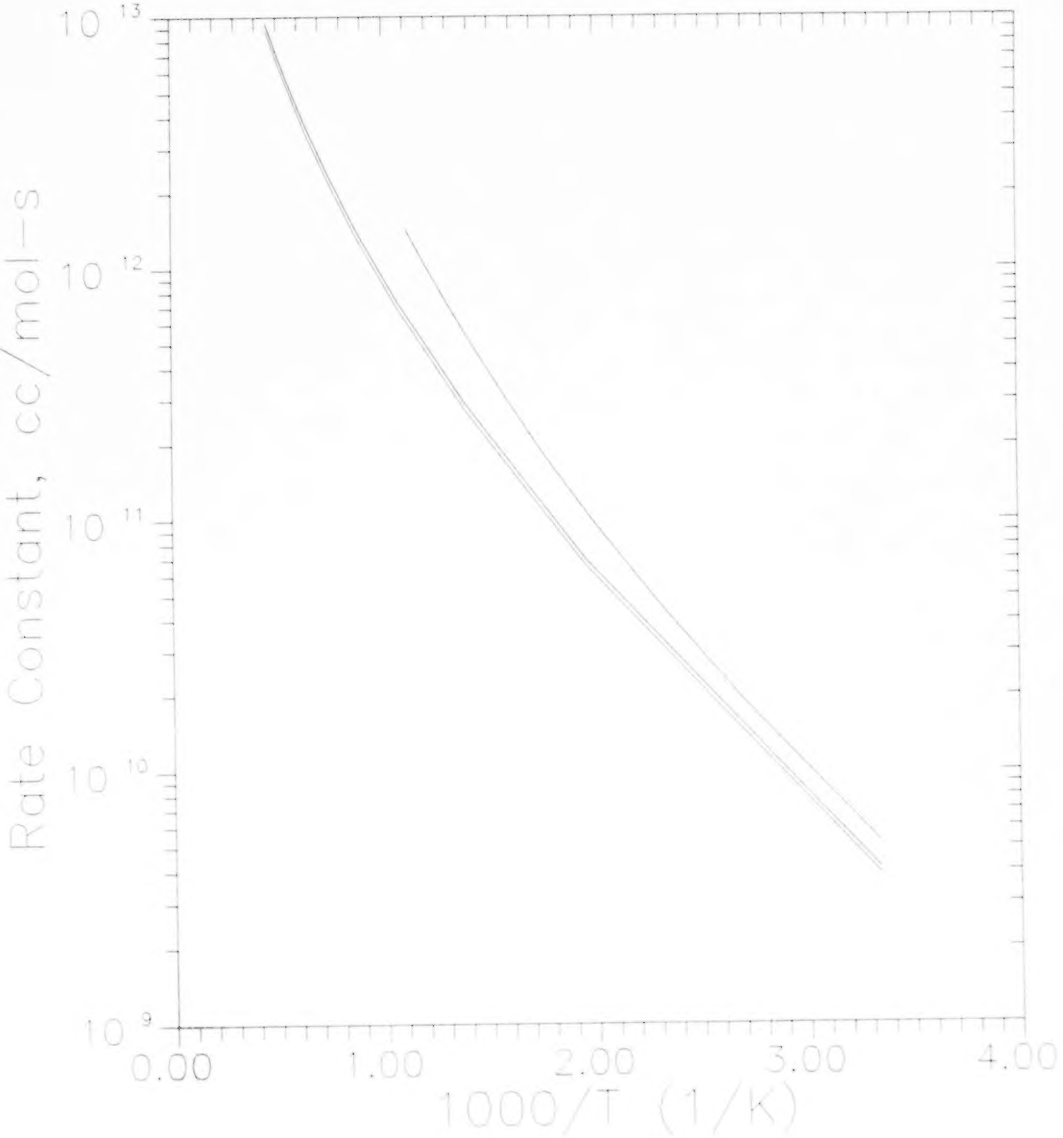
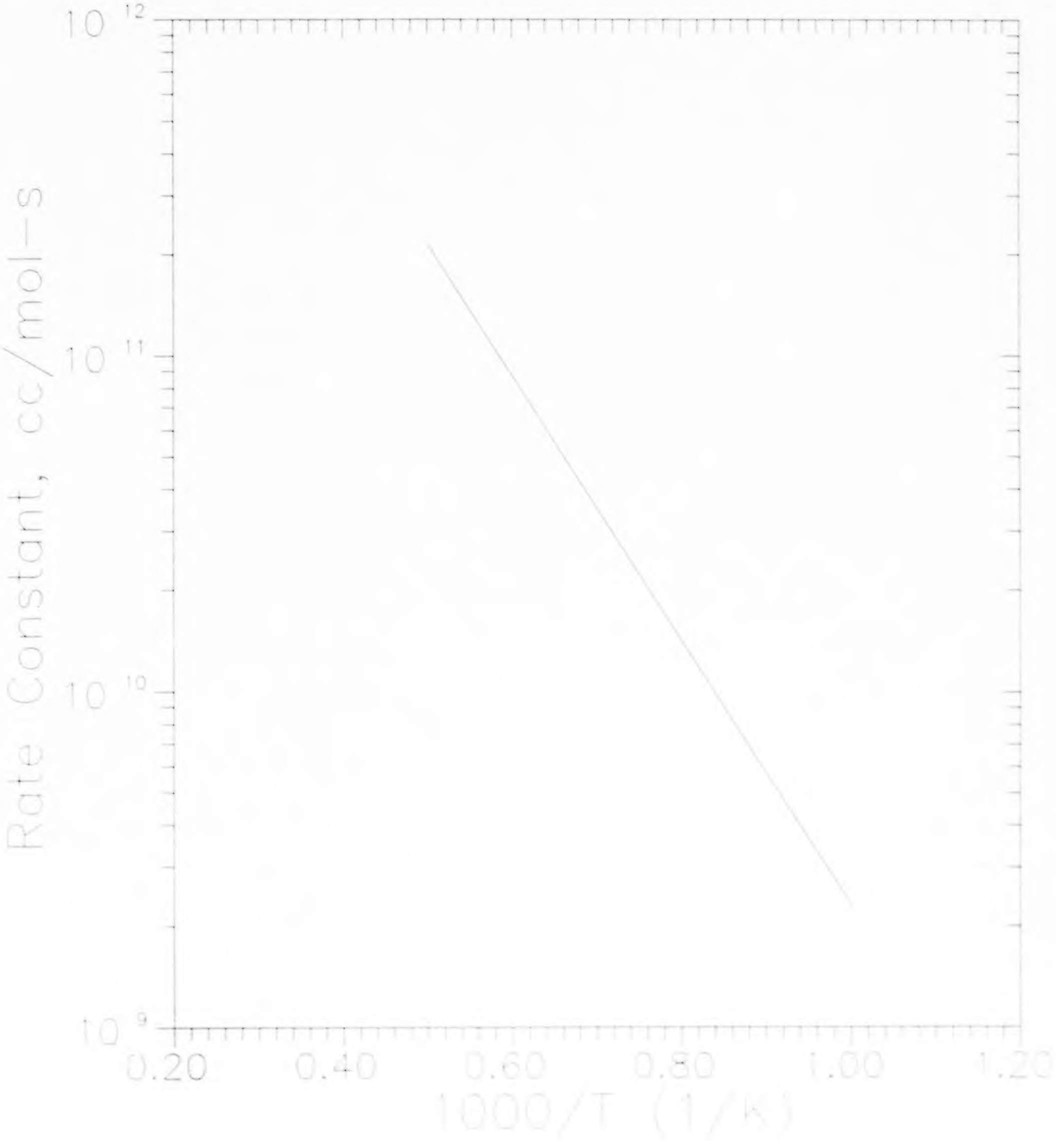



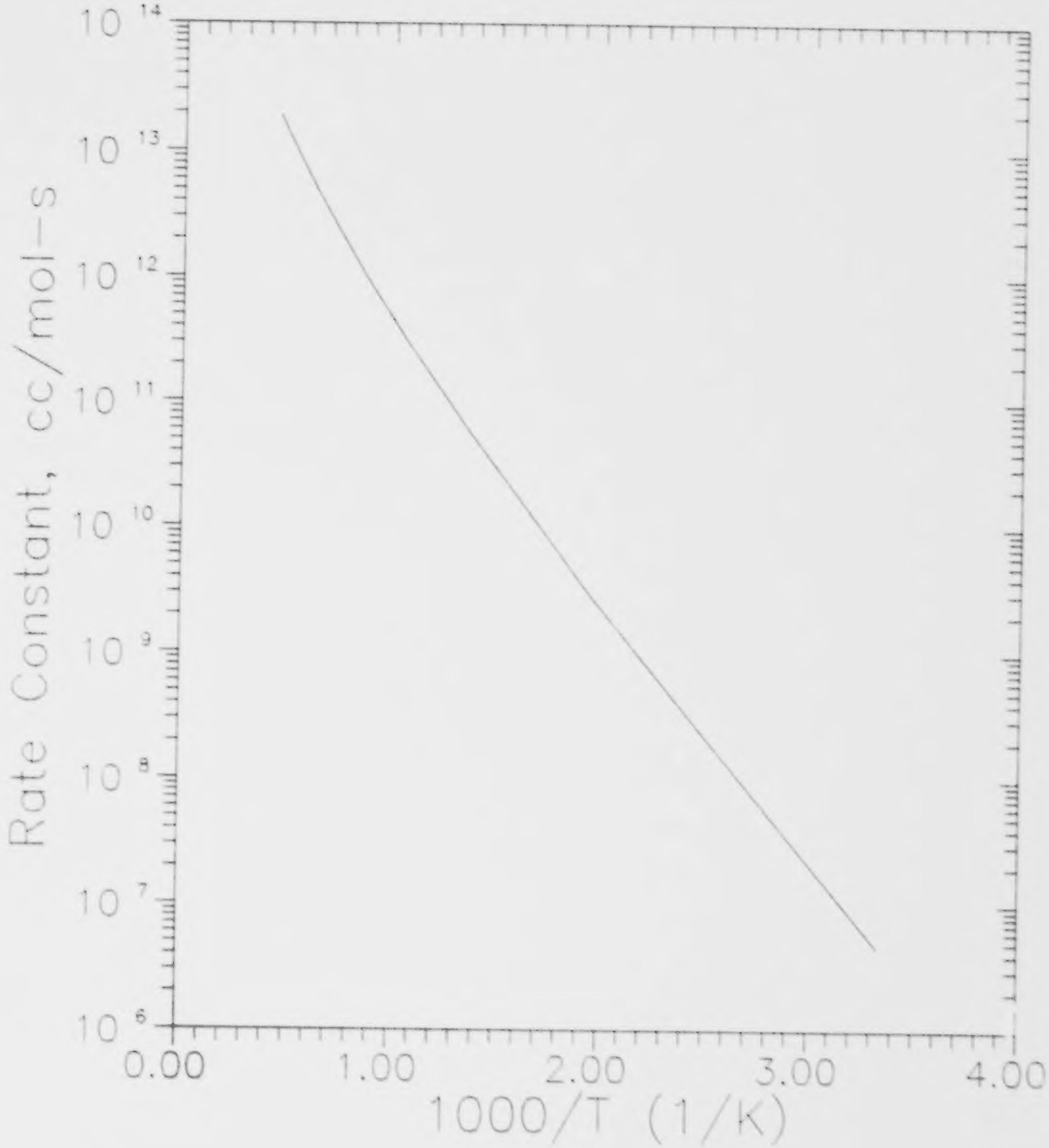
**CH4 + O2 = CH3 + HO2**



**CH4 + HO = CH3 + H2O**



**$CH_4$ + $HO_2$ = $CH_3$ + $H_2O_2$**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10 10
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10 8
10 7
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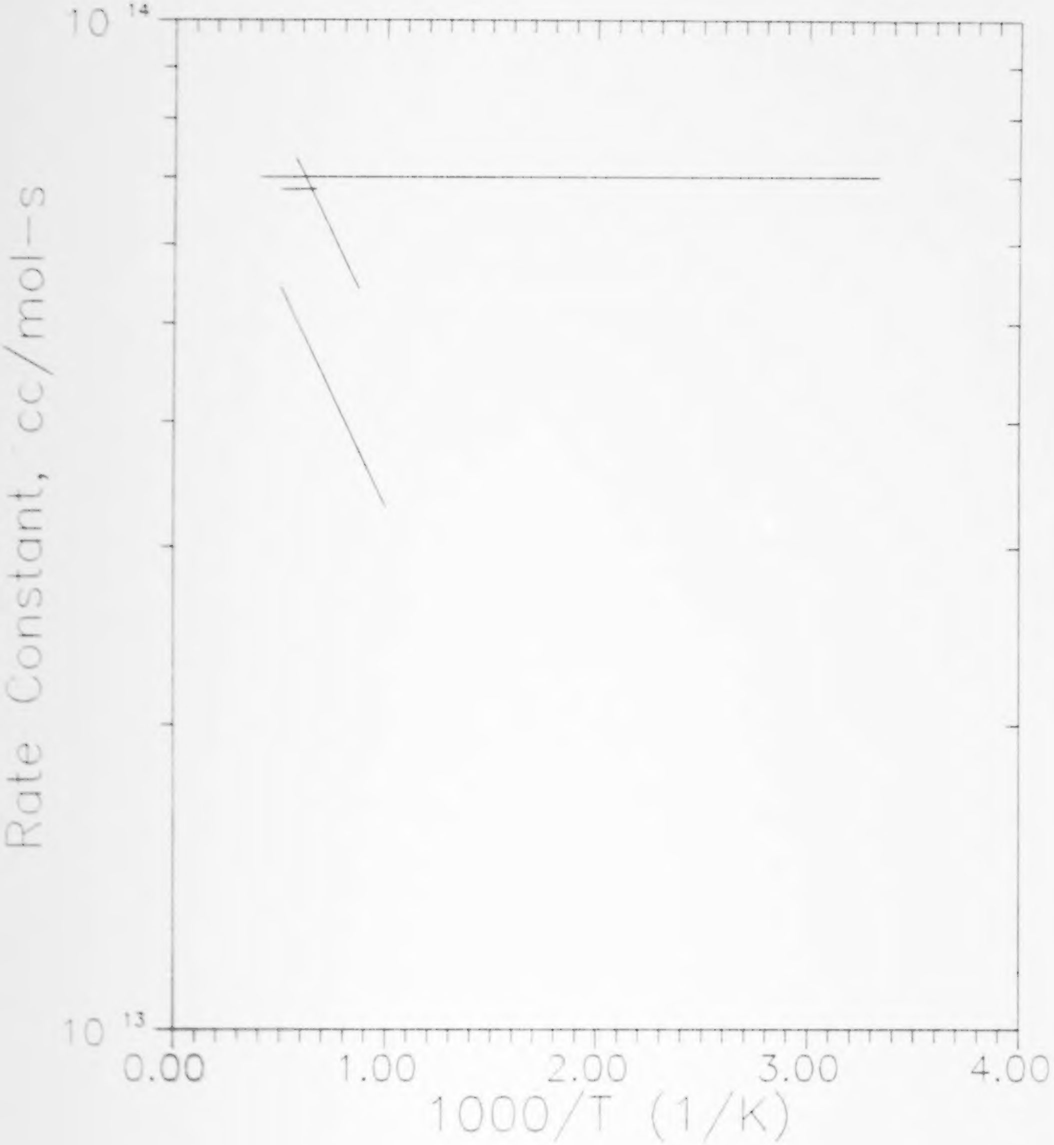
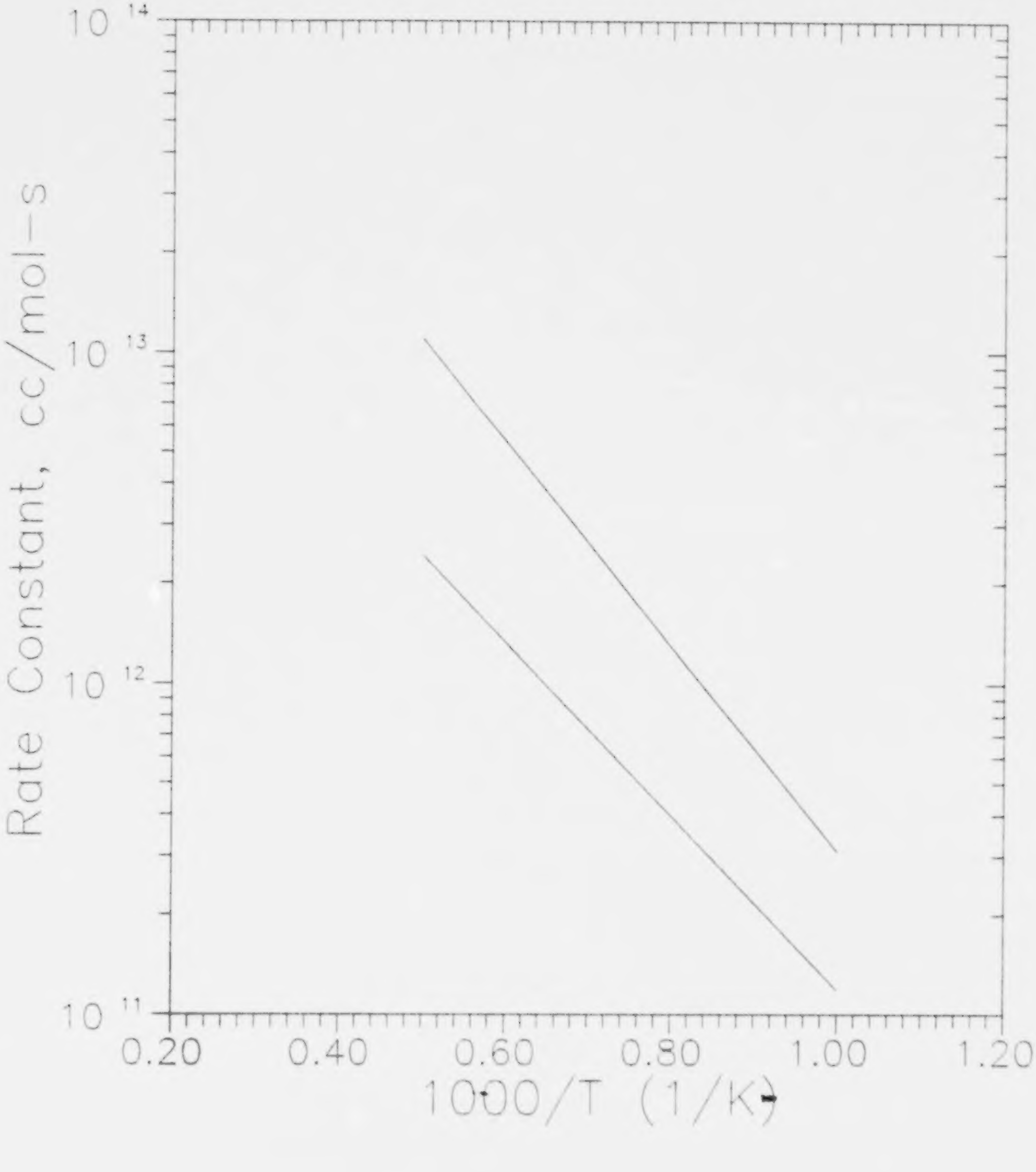
3.00
4.00
1000/T (1/K)

**CH4 + O = CH3 + HO**



**CH3 + O = CH2O + H**



Rate Constant, cc/mol-s
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$10^{13}$
$10^{12}$
$10^{11}$
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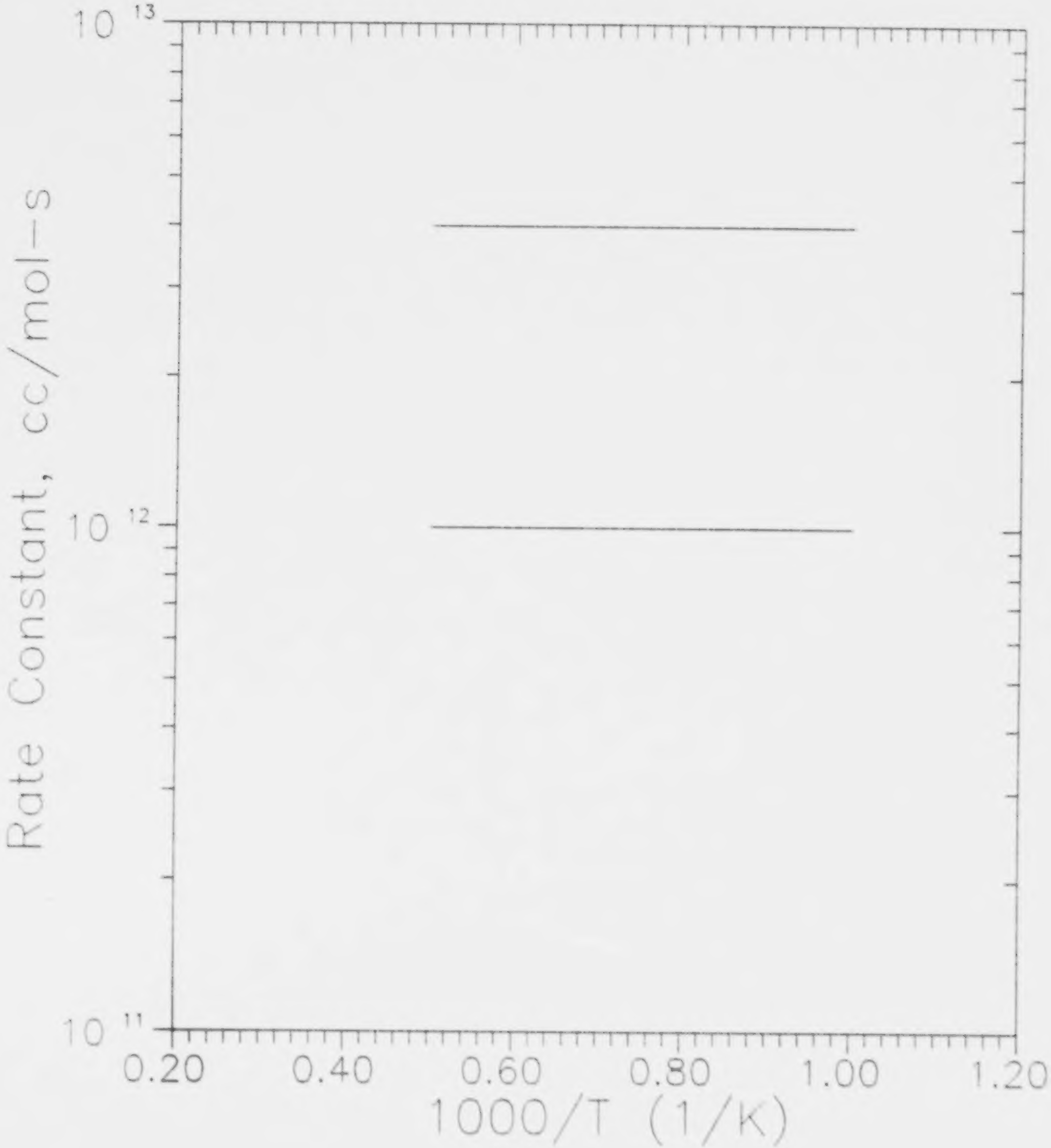
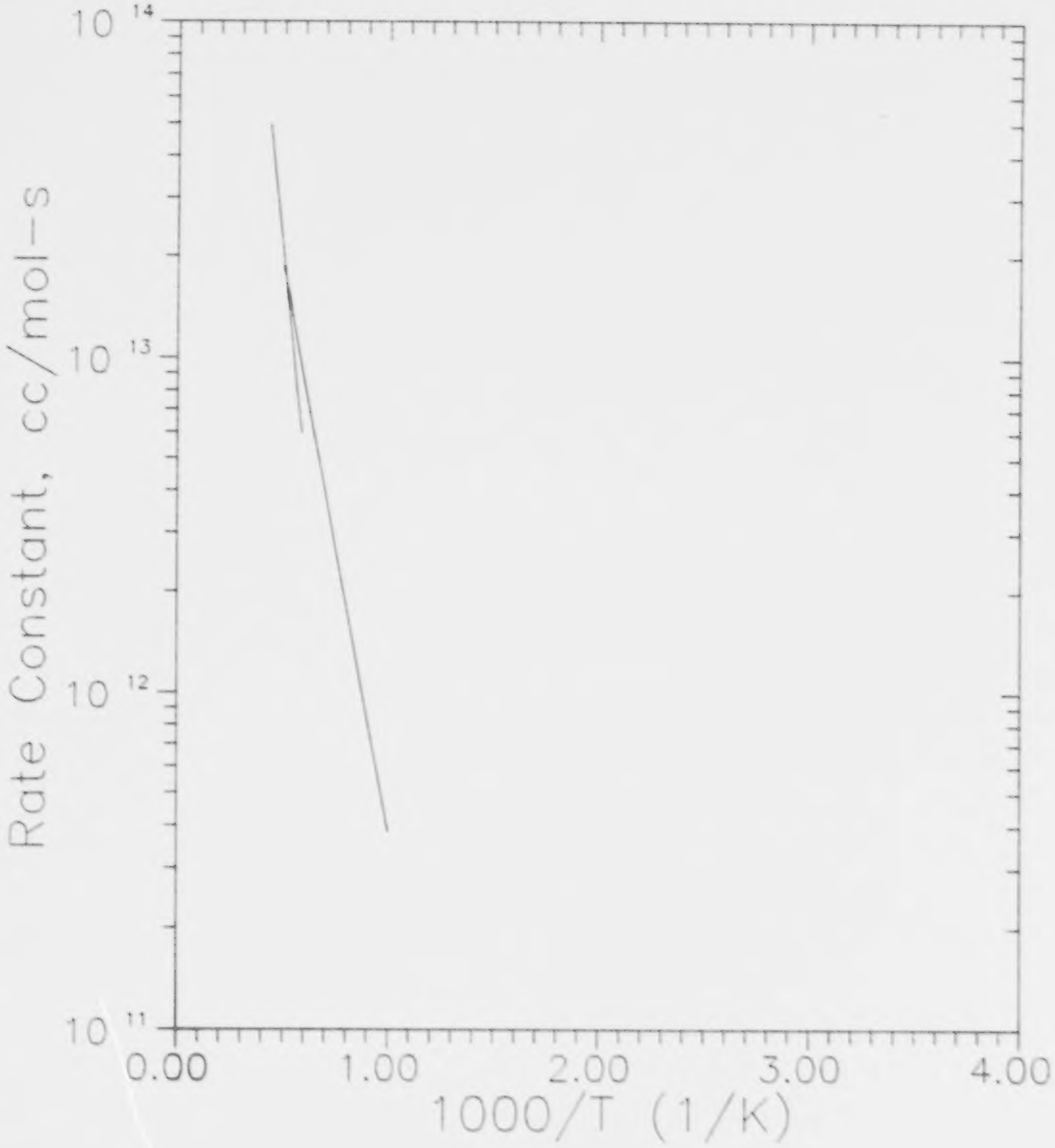
0.60
0.80
1.00
1.20
1000/T (1/K)

**$CH_3$ + O = $CH_2$ + HO**



**CH3 + HO = CH2O + H2**


10 14
10 13
10 12
10 11
Rate Constant, cc/mol-s
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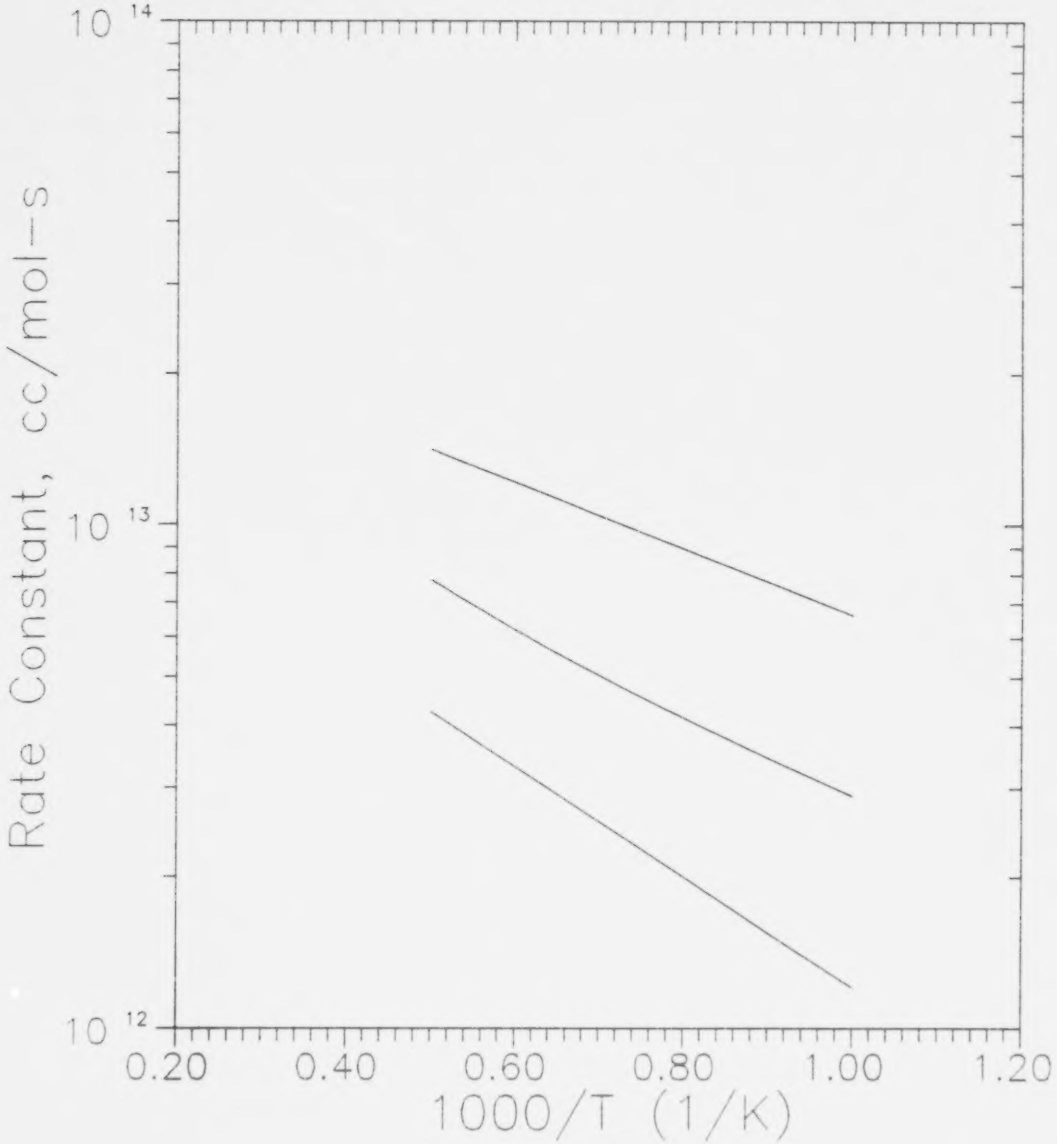
1.00
2.00
3.00
4.00
1000/T (1/K)

**CH3 + HO = CH3O + H**



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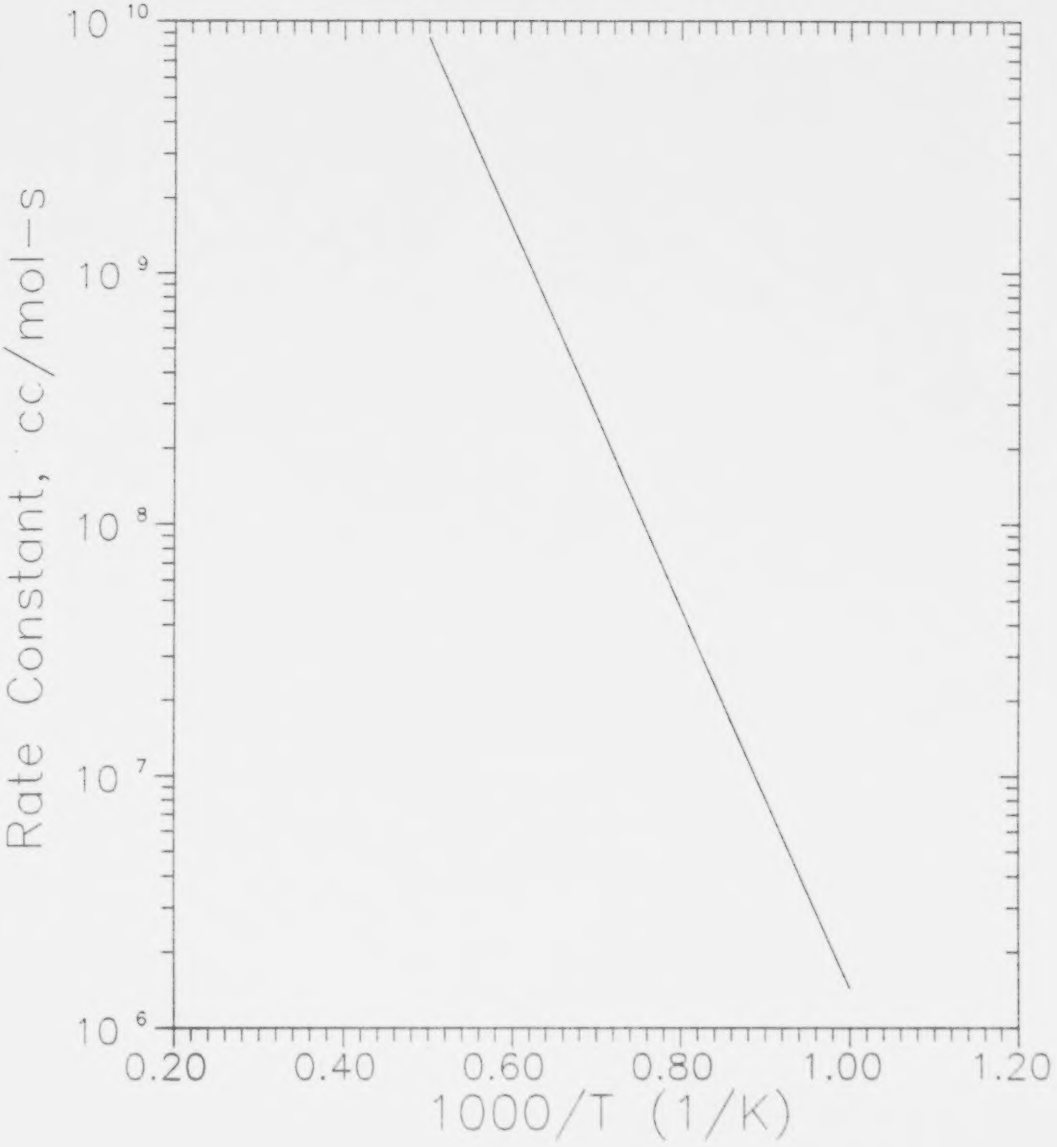
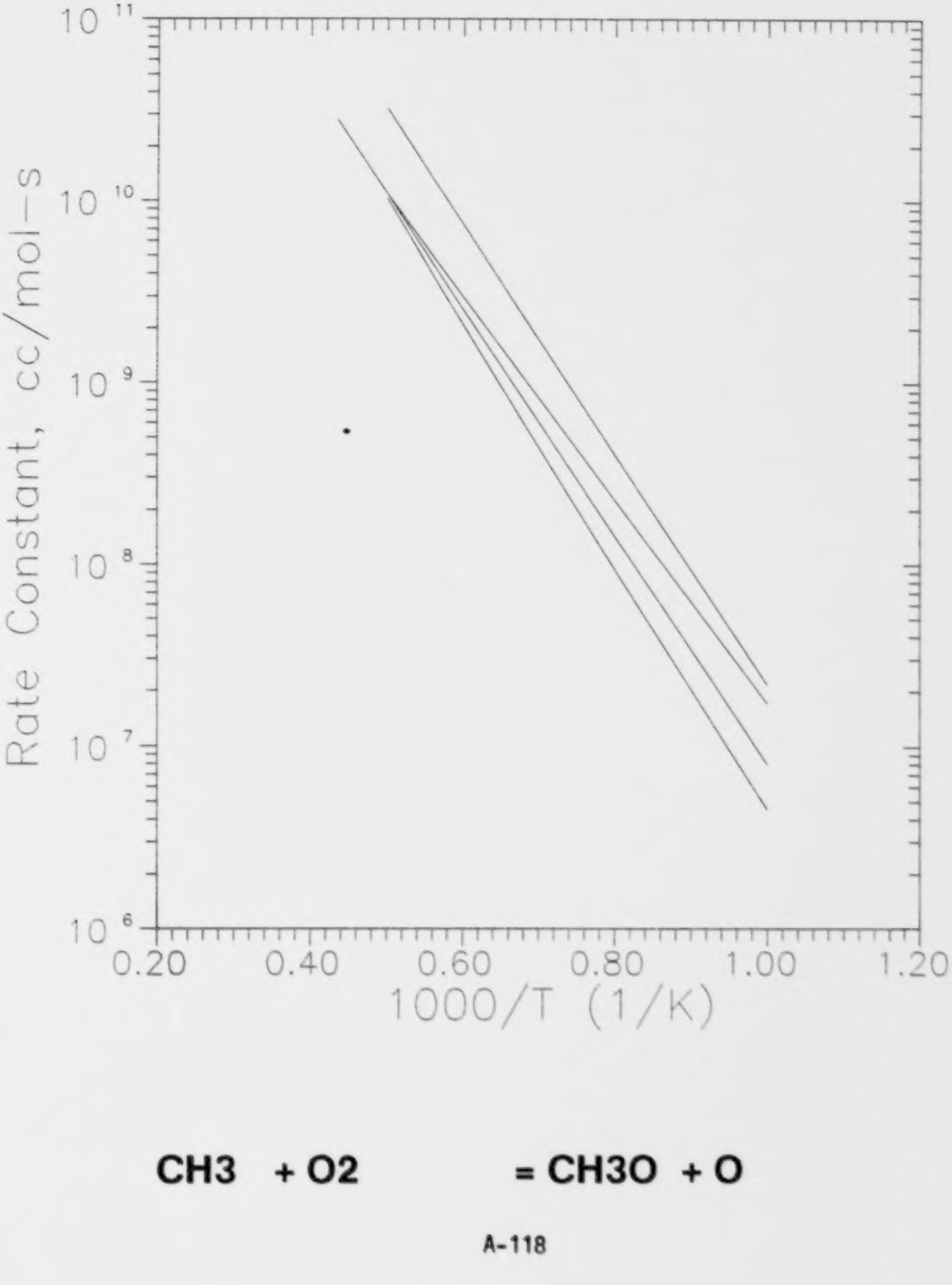


**CH3 + O2 = CH2O + HO**



Rate Constant, cc/mol-s
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10 7
10 6
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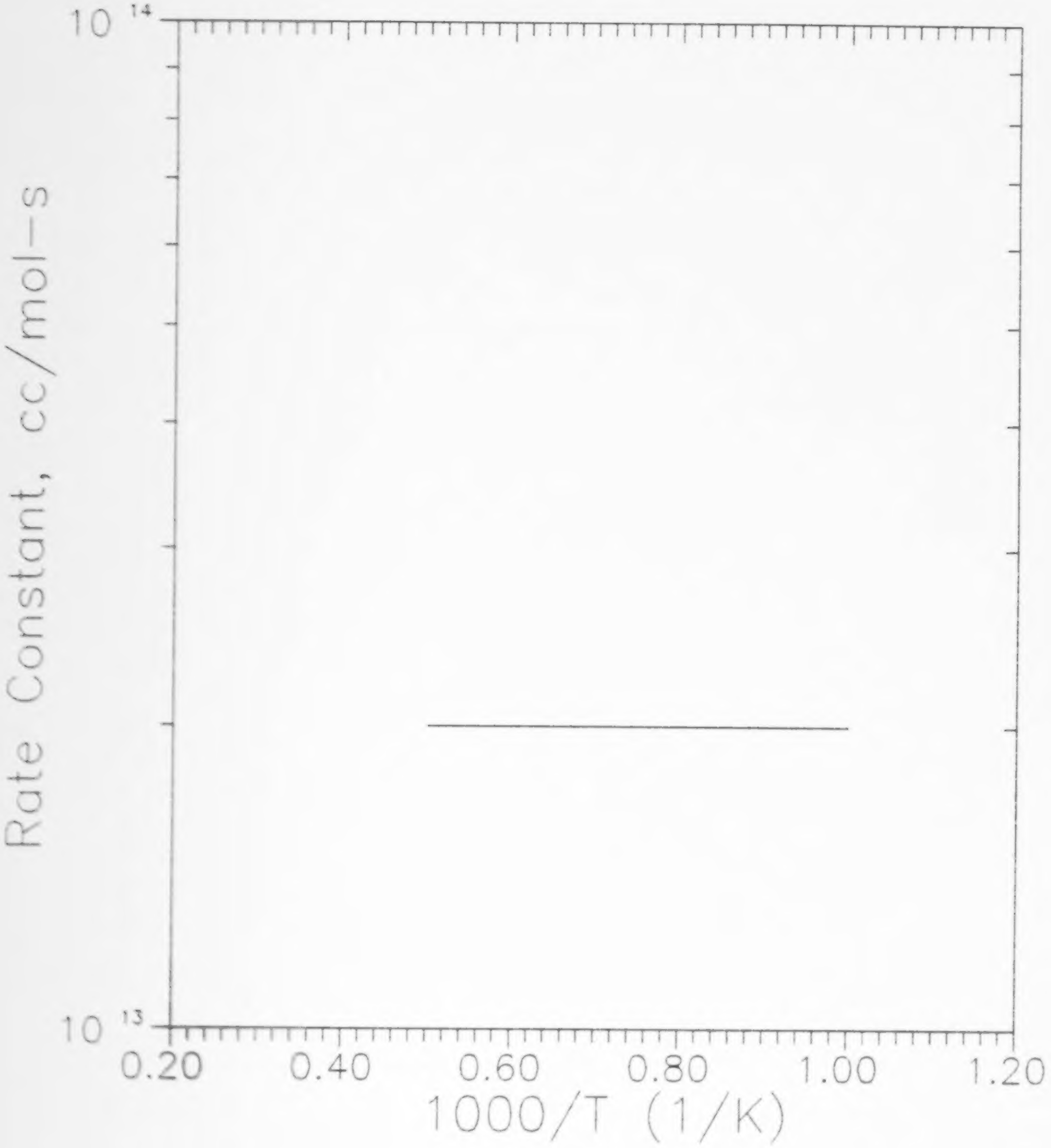
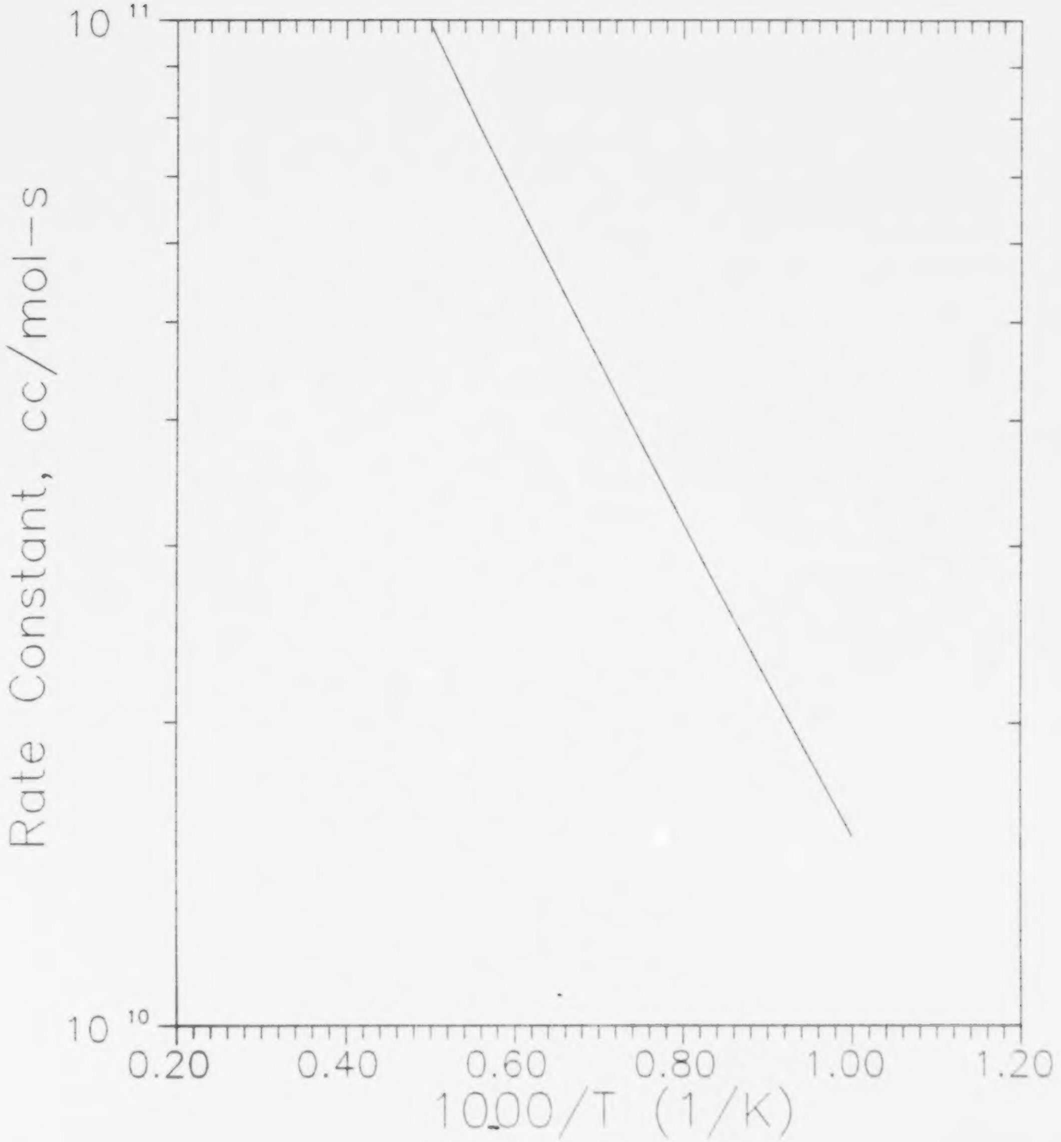
0.60
0.80
1.00
1.20
1000/T (1/K)

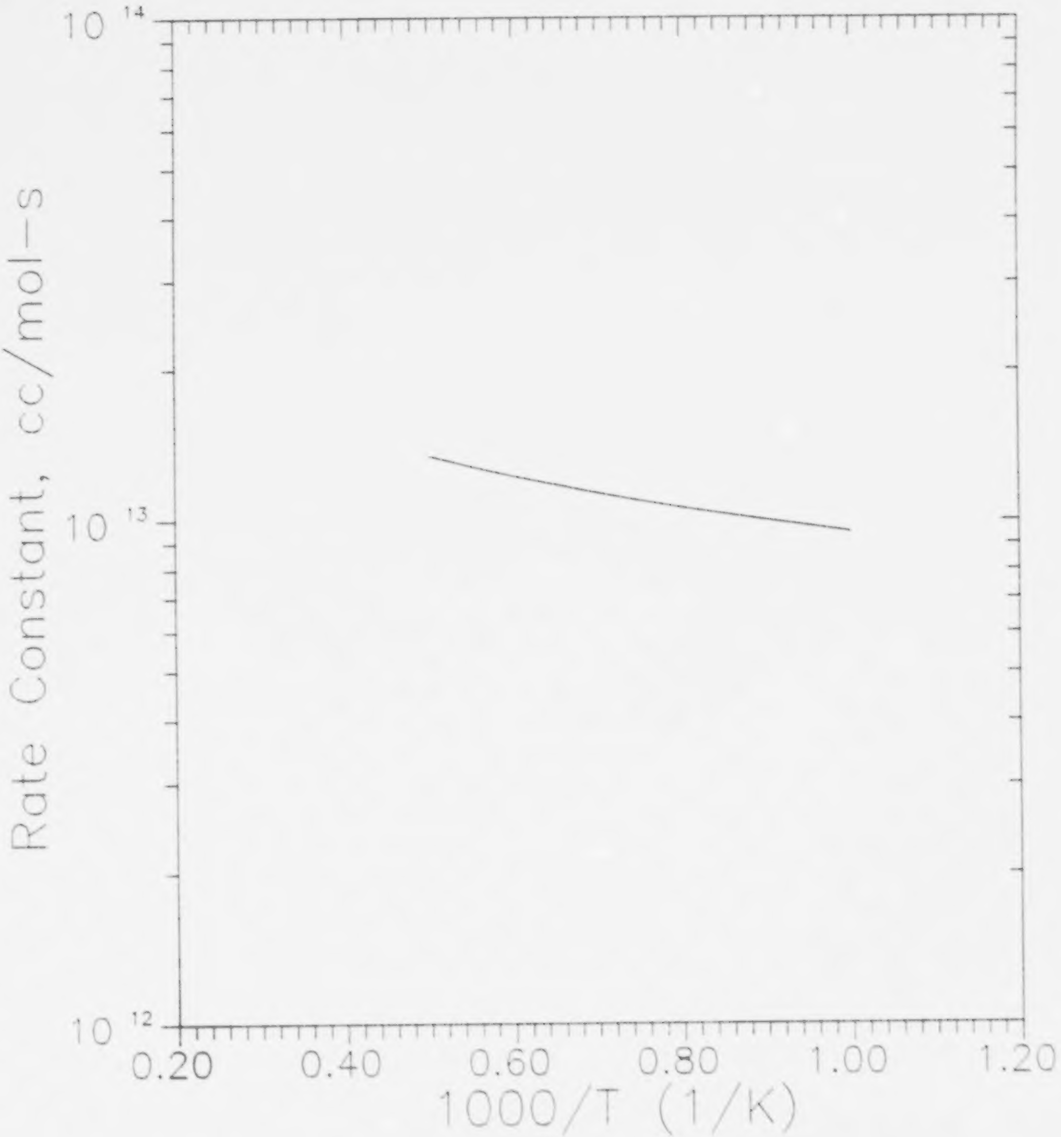
**CH3 + O2 = CH3O + O**



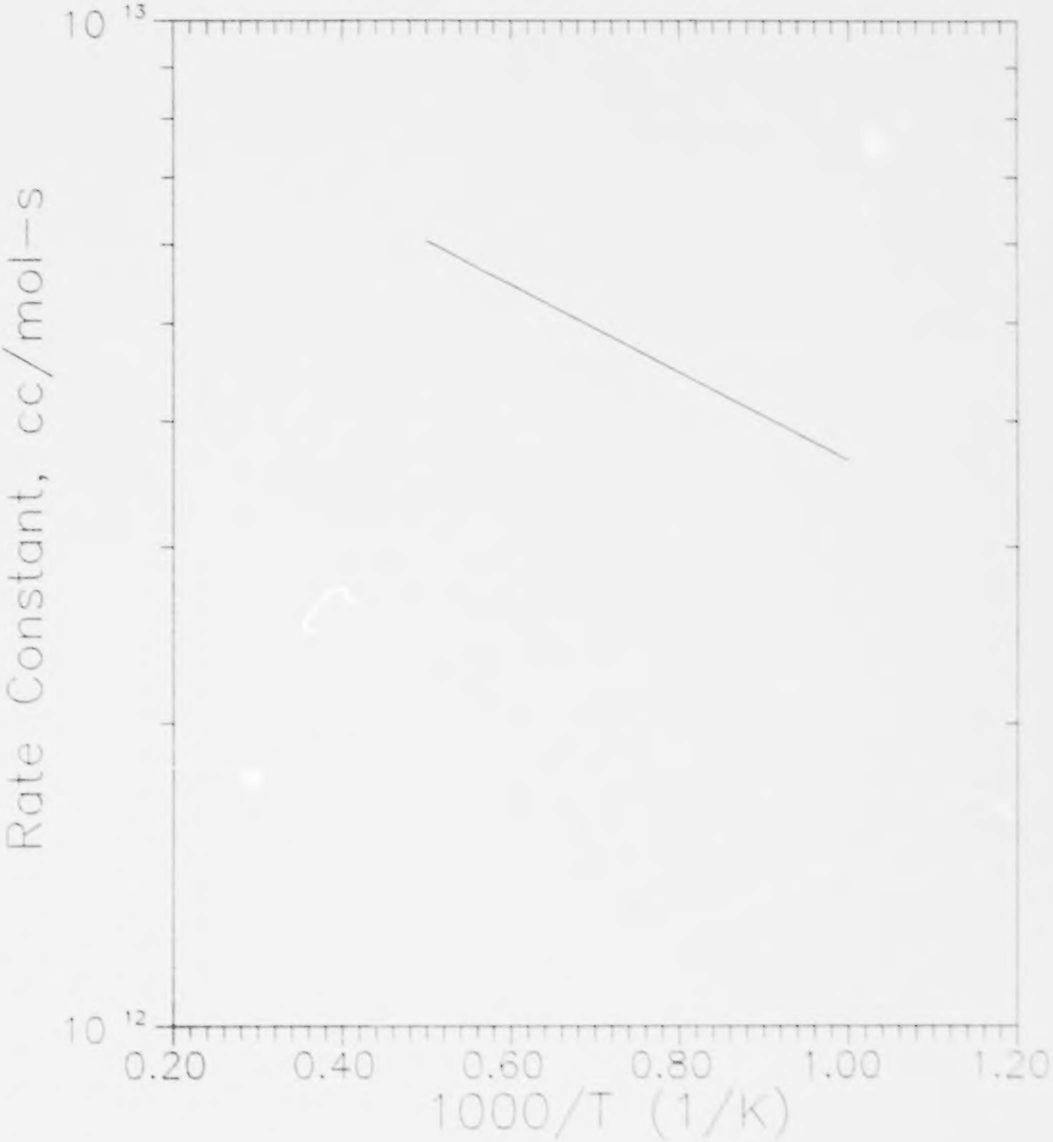
**CH3 + HO2 = CH3O + HO**



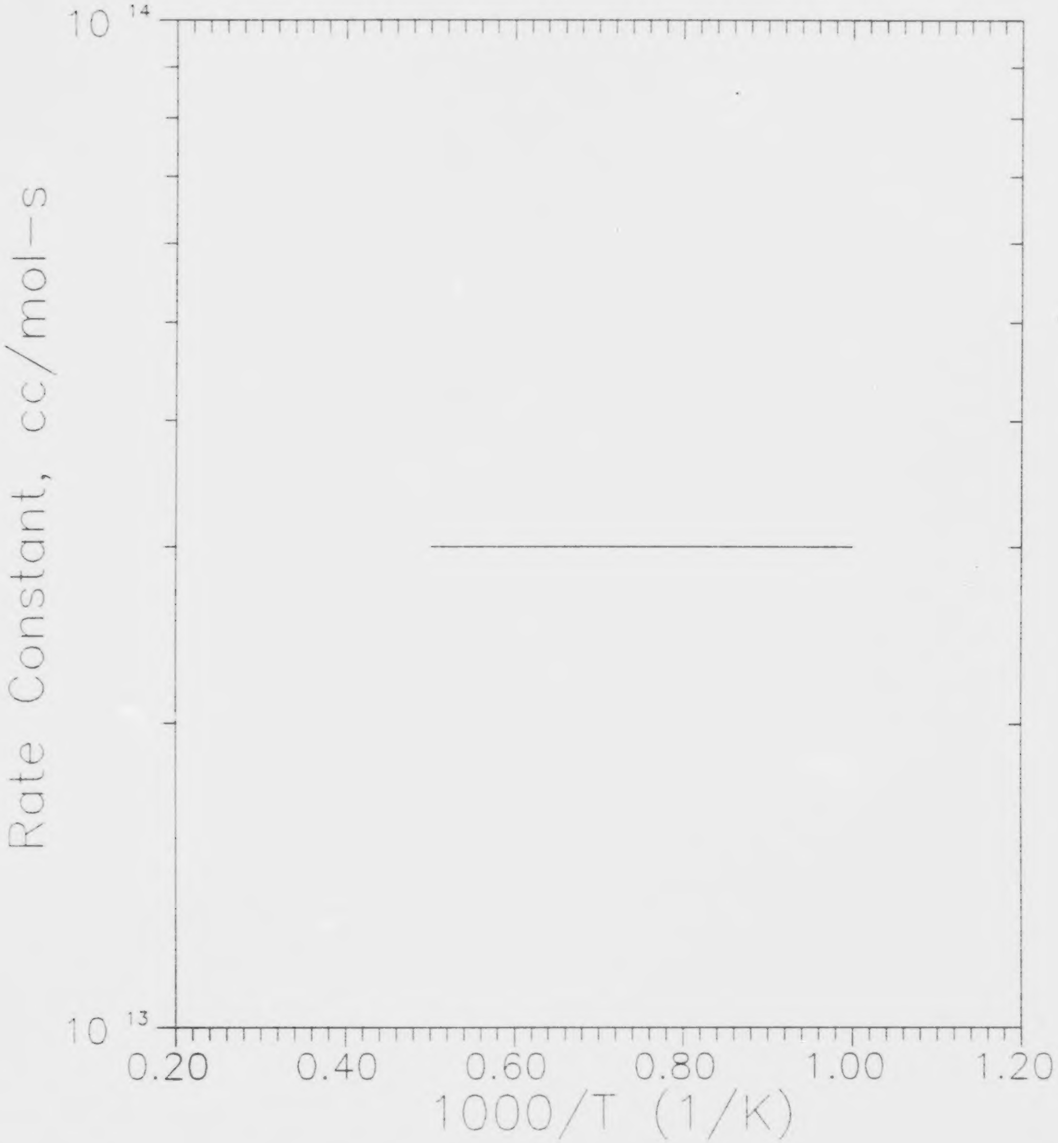
**CH3 + CH2O = CHO + CH4**



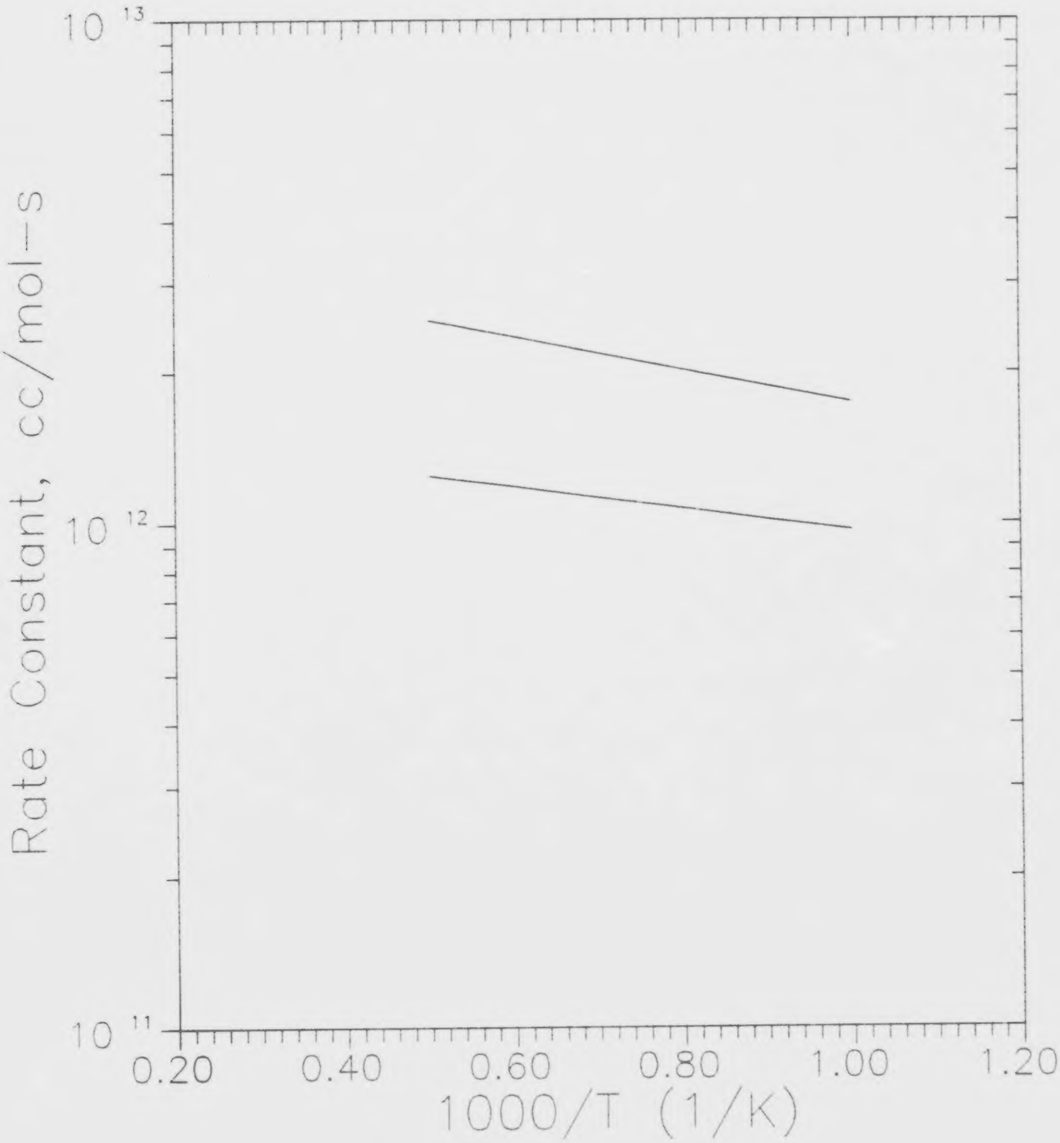
**CH3 + CHO = CO + CH4**



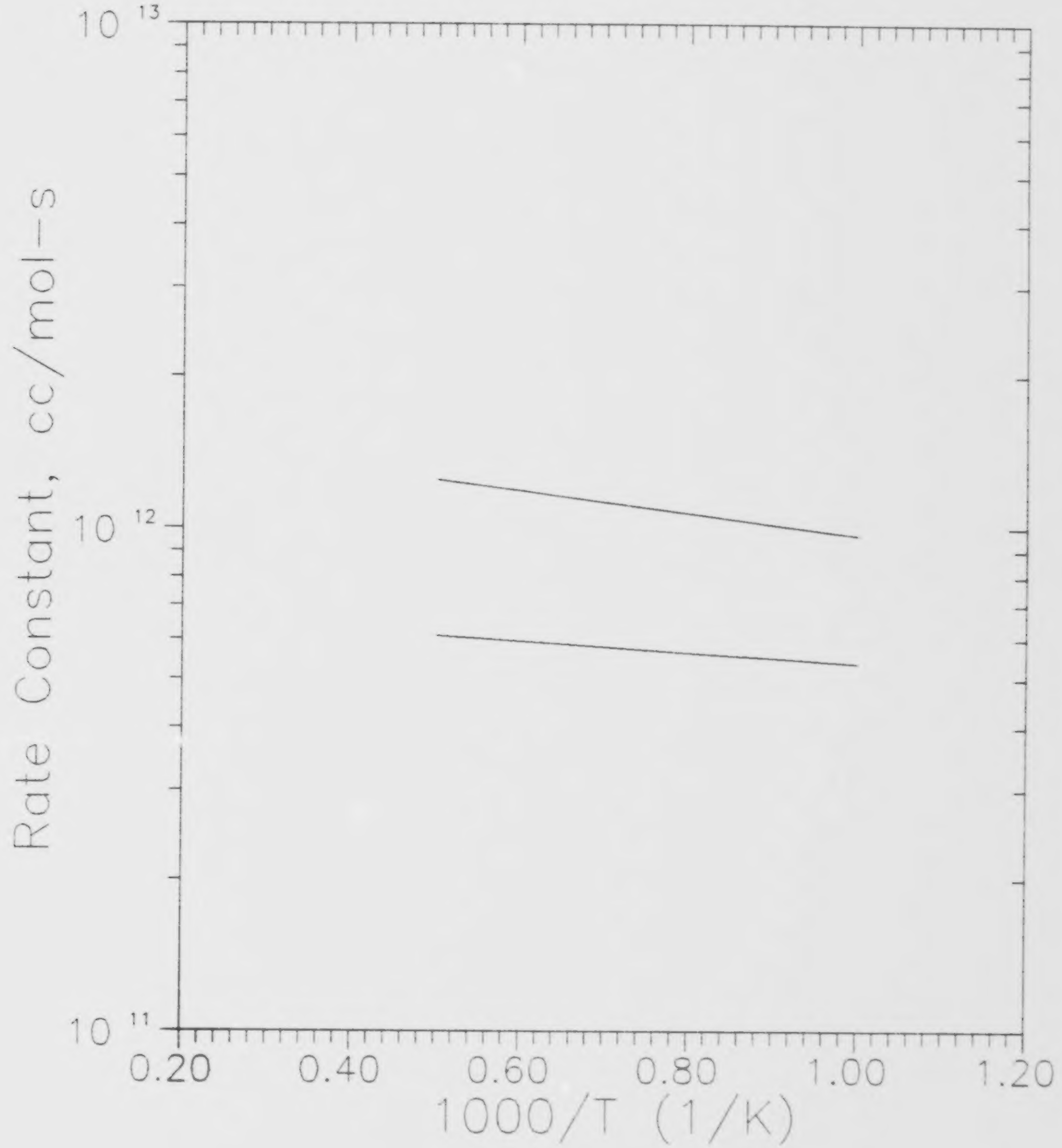
**CH2 + CHCO = C2H + CH2O**



**$CH_2$ + CHCO = $C_2H_3$ + CO**


10 13
10 12
10 11
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O2 = CO2 + H + H**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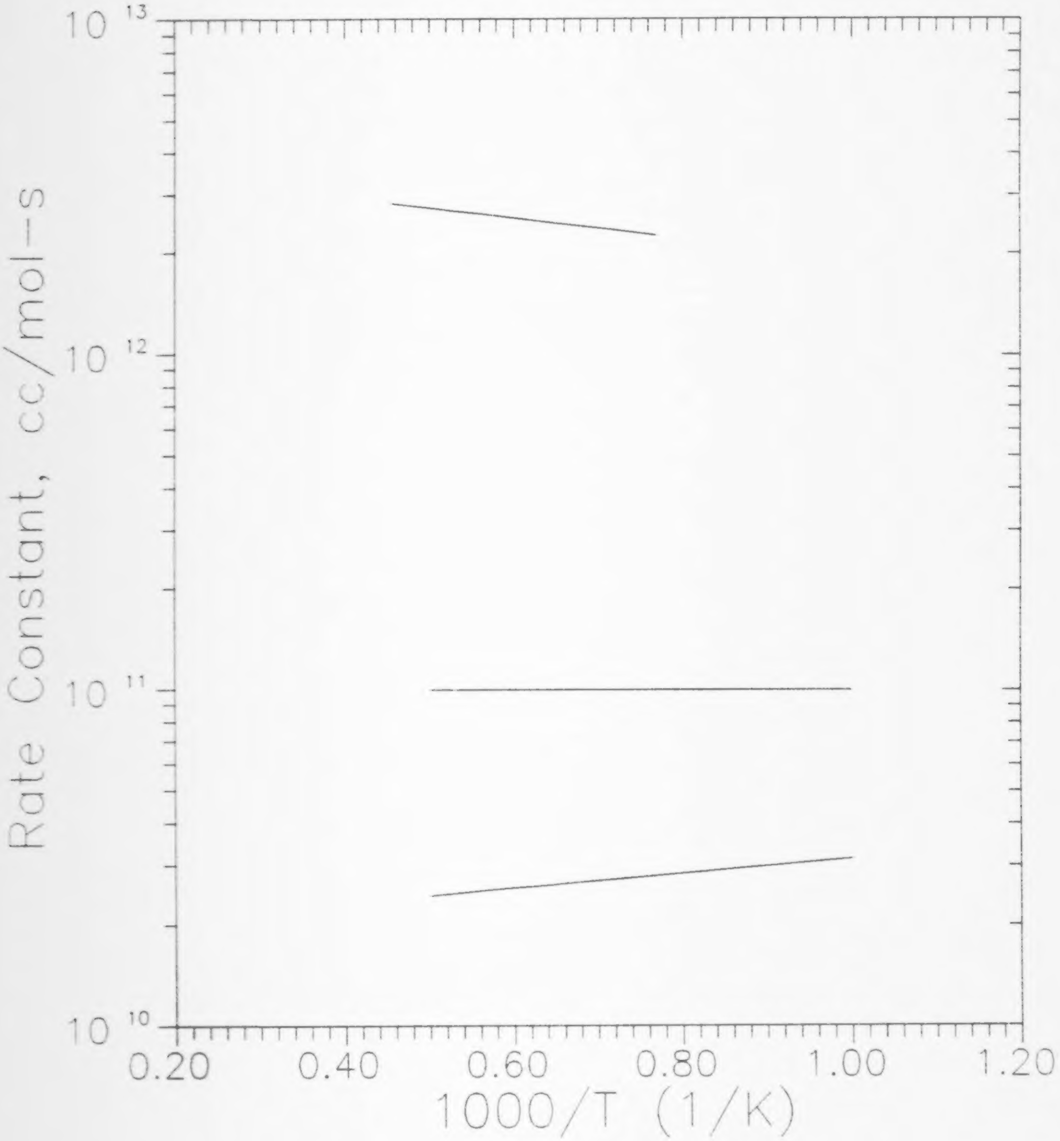
10 12
10 11
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O2 = CO2 + H2**



Rate Constant, cc/mol-s
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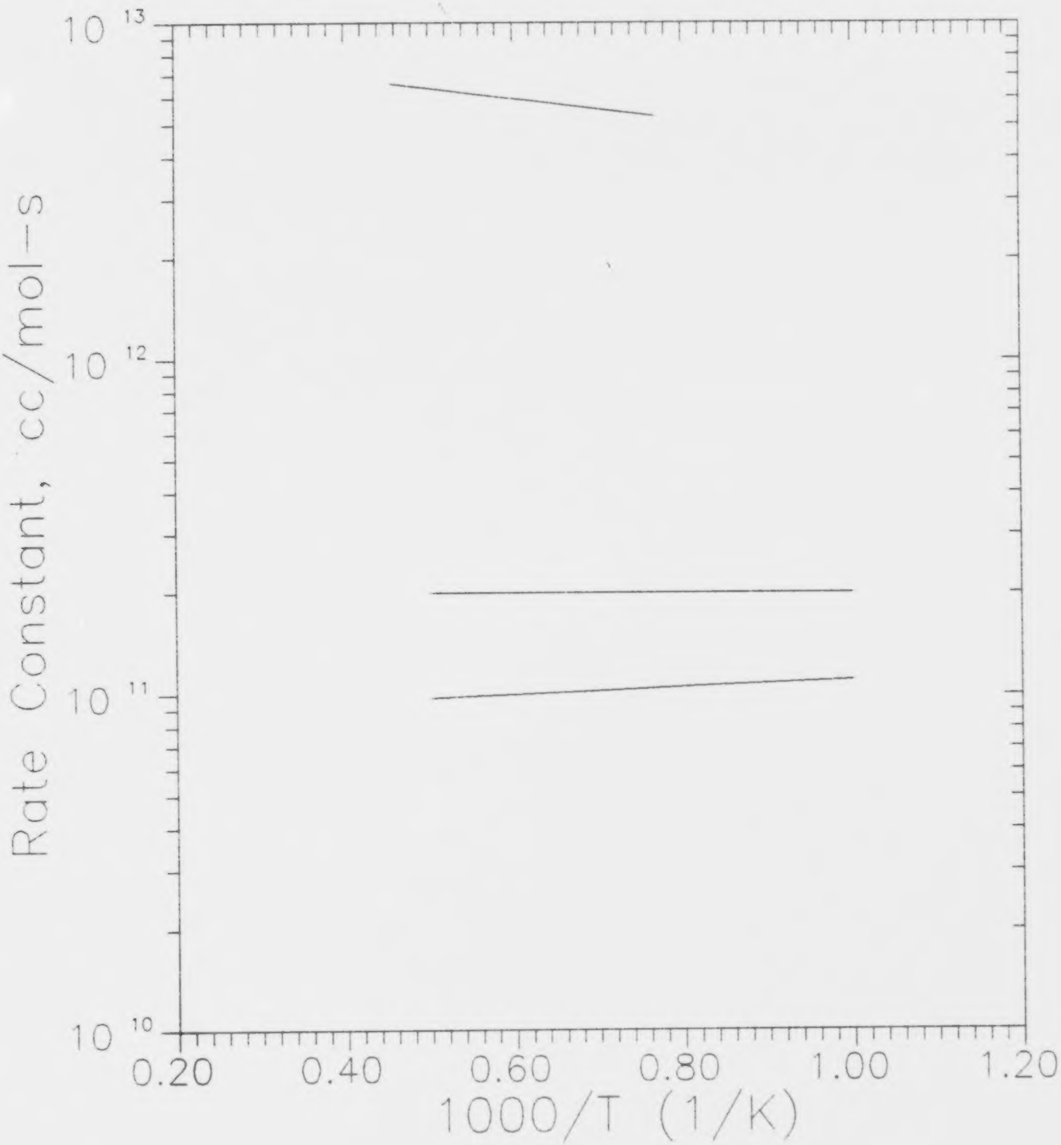
$10^{12}$
$10^{11}$
$10^{10}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O2 = CO + H2O**


Rate Constant, cc/mol-s
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$10^{12}$
$10^{11}$
$10^{10}$
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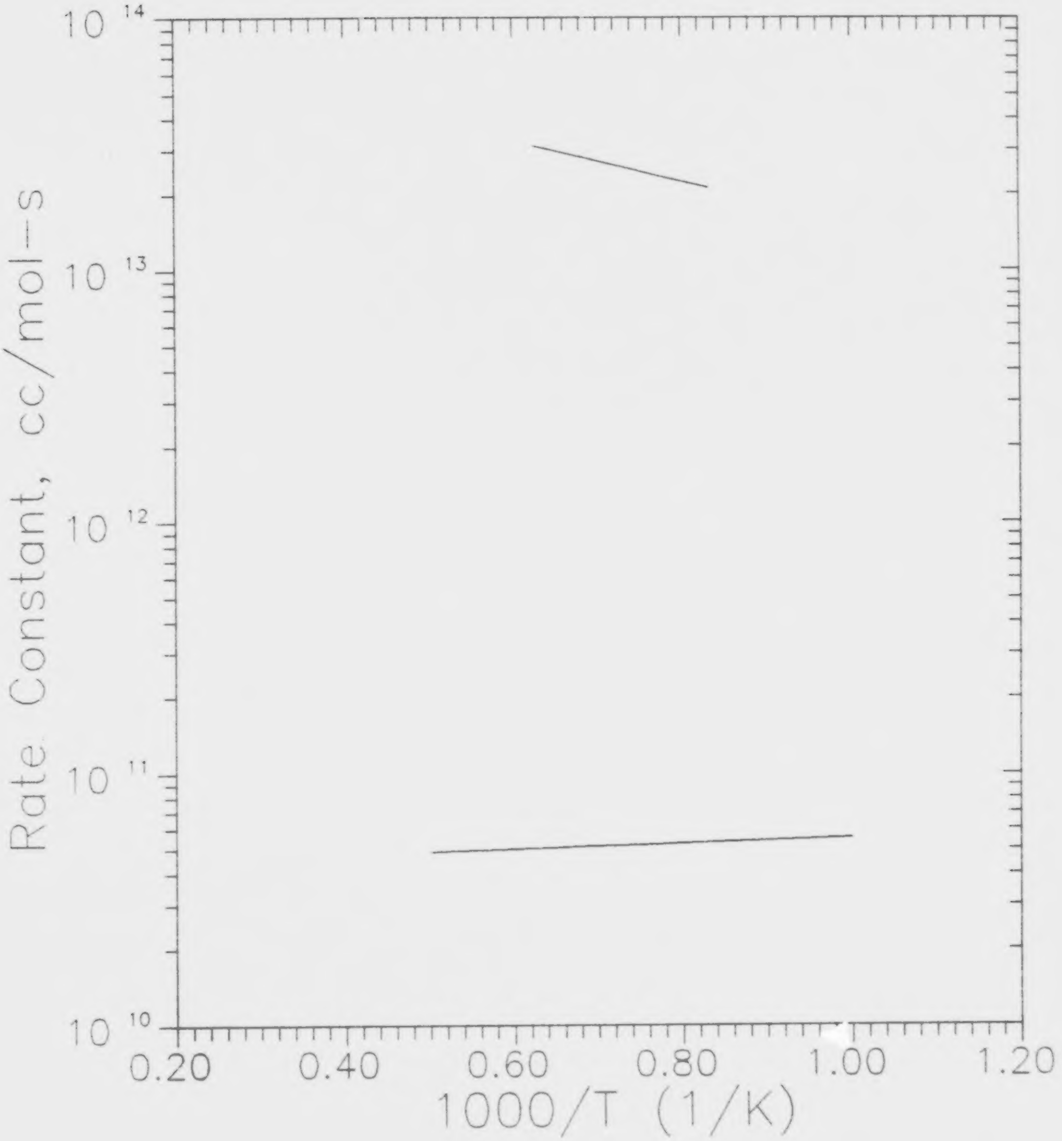
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O2 = CO + HO + H**



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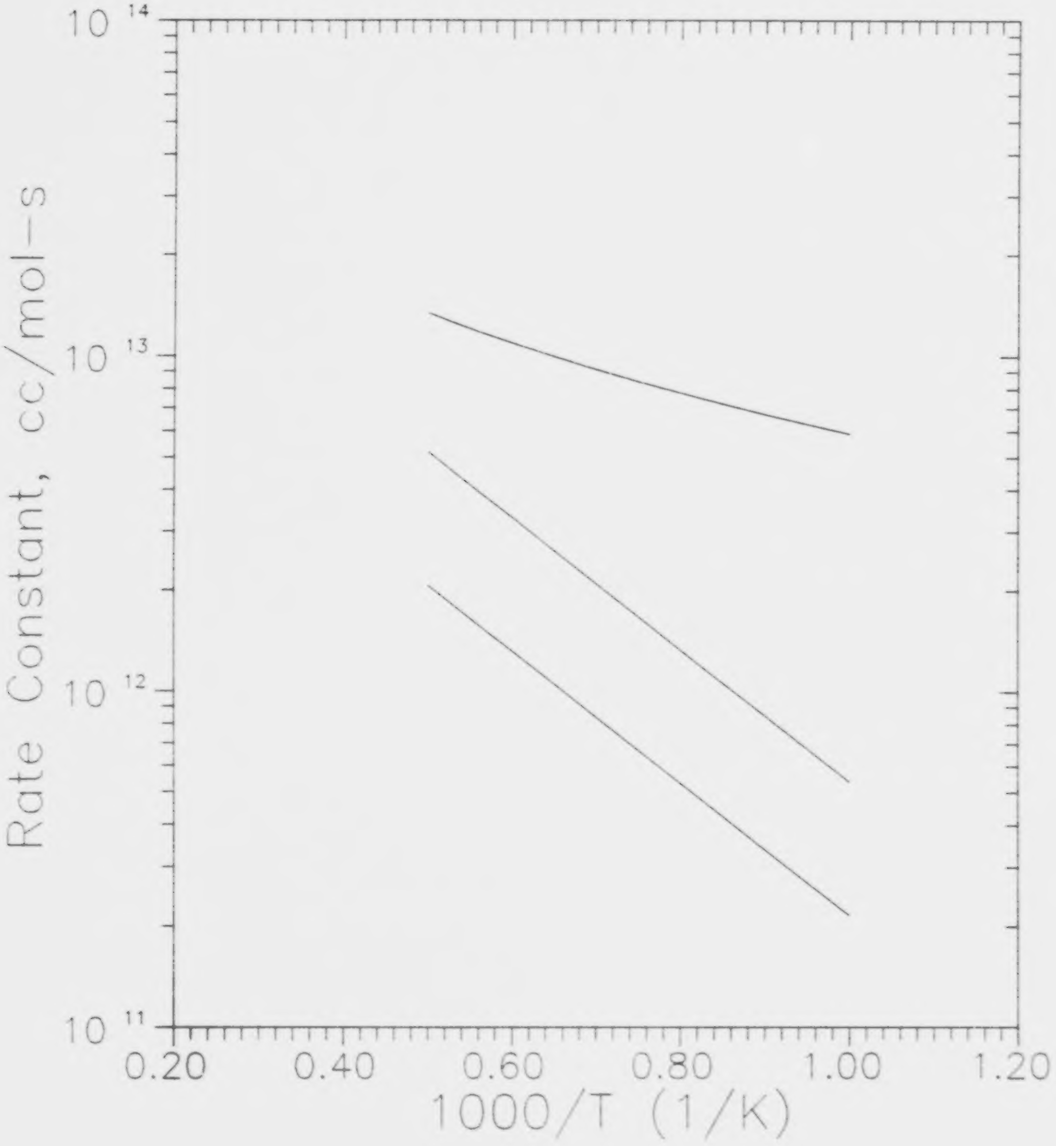
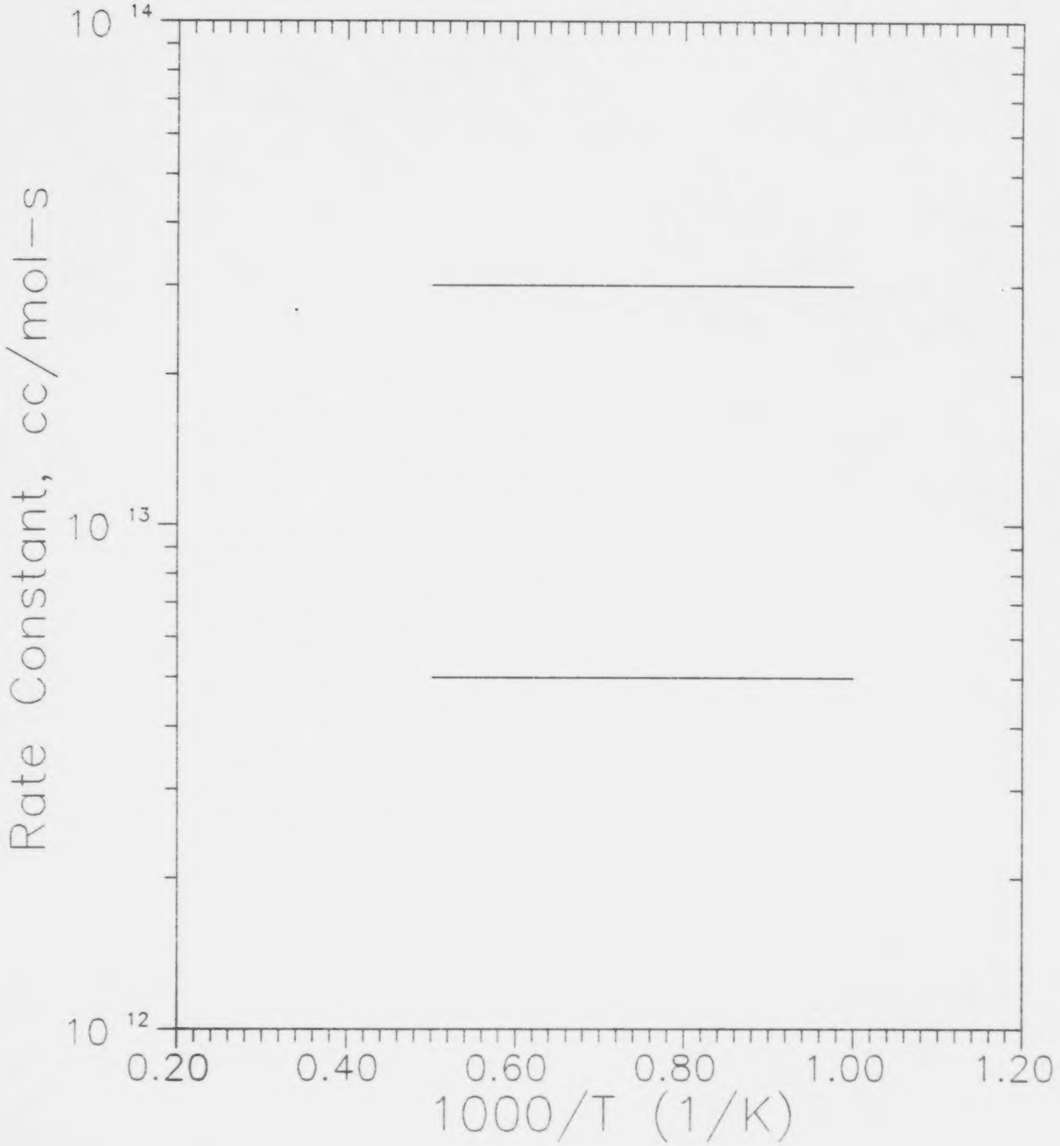
10 12
10 11
10 10
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)
Rate Constant, cc/mol-s

**CH2 + O2 = CHO + HO**



Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O2 = CH2O + O**


10 14
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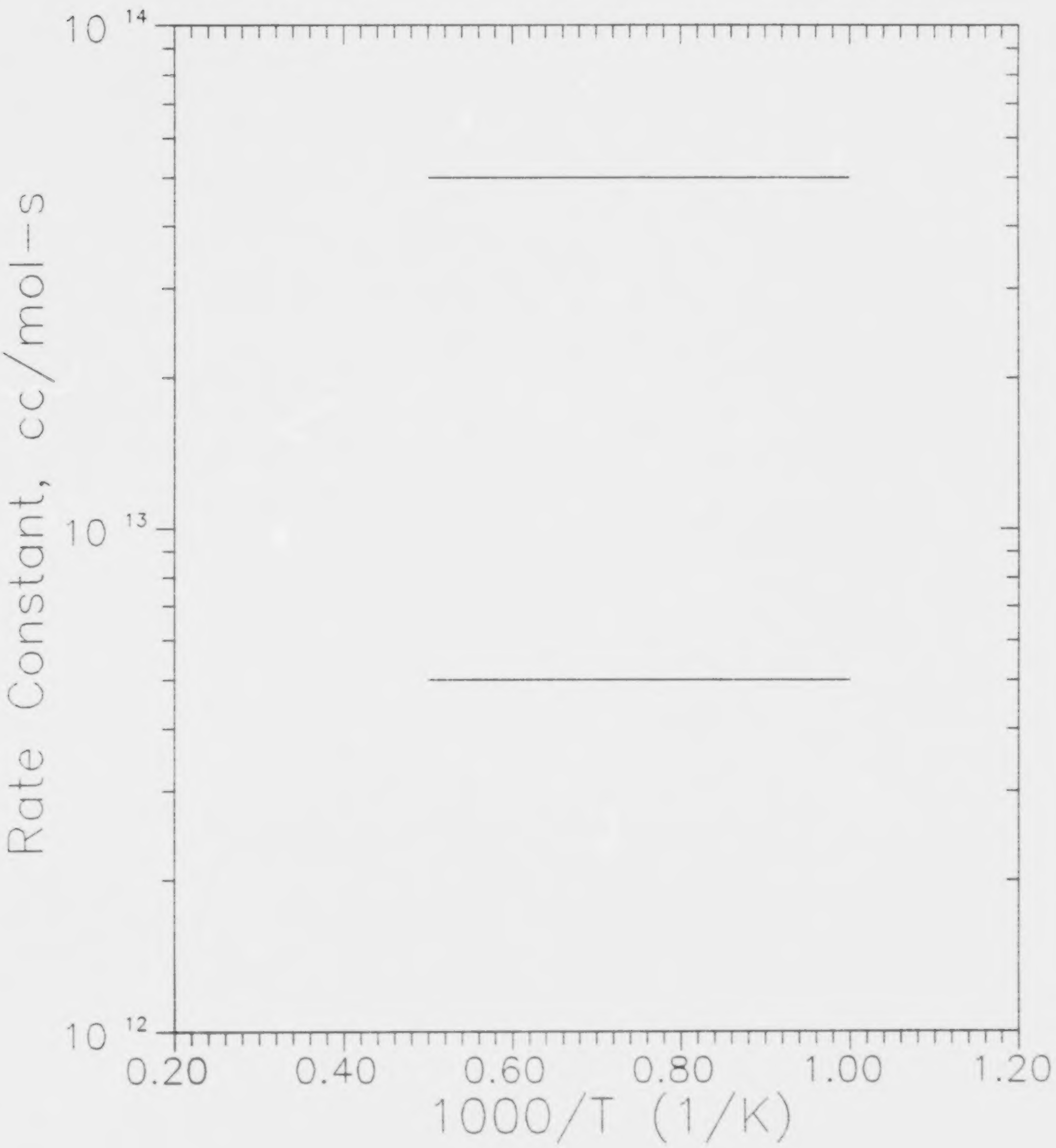
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O = CO + H + H**



Rate Constant, cc/mol-s
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10 12
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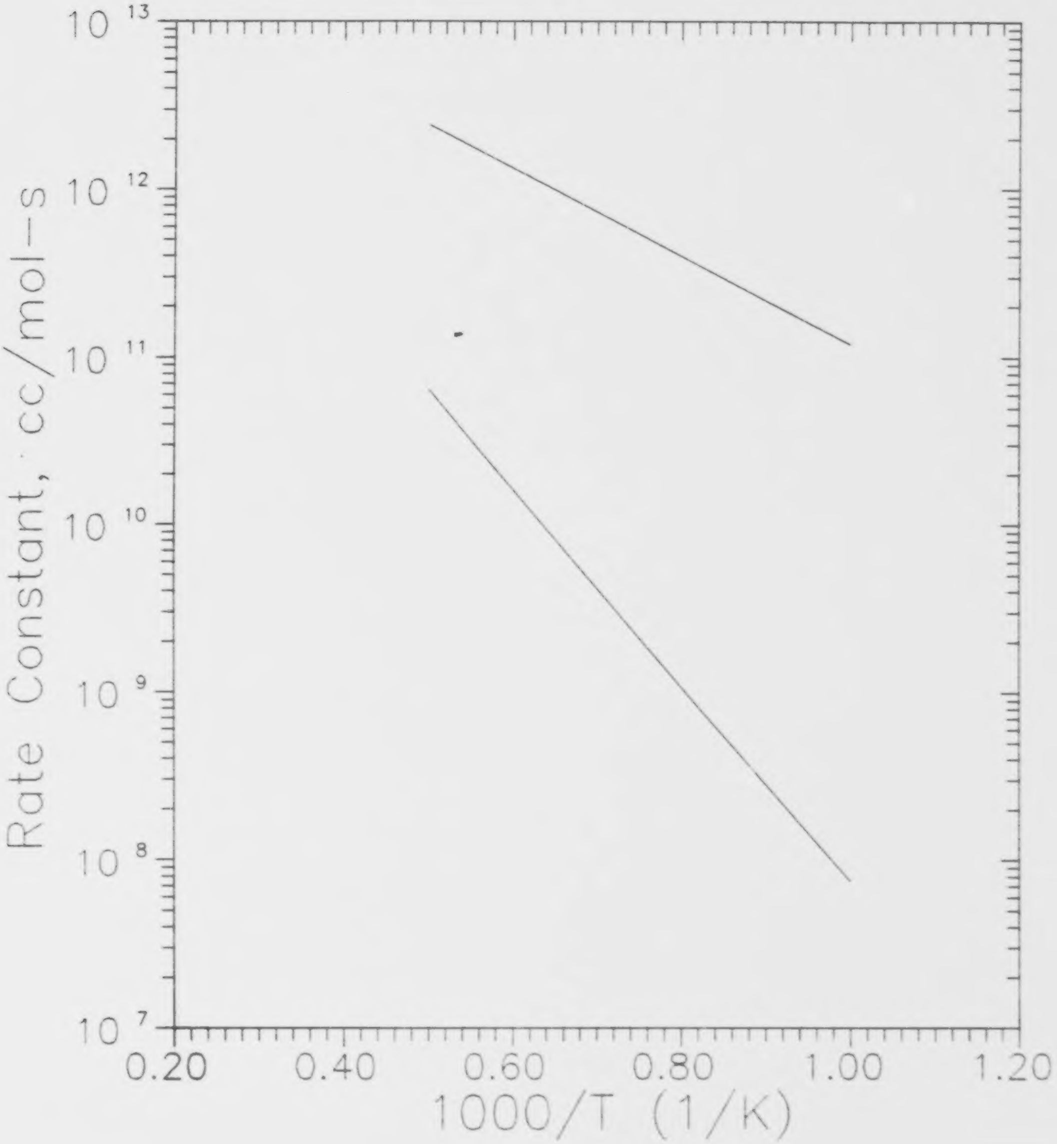
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O = CO + H2**



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10 9
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10 7
Rate Constant, cc/mol-s
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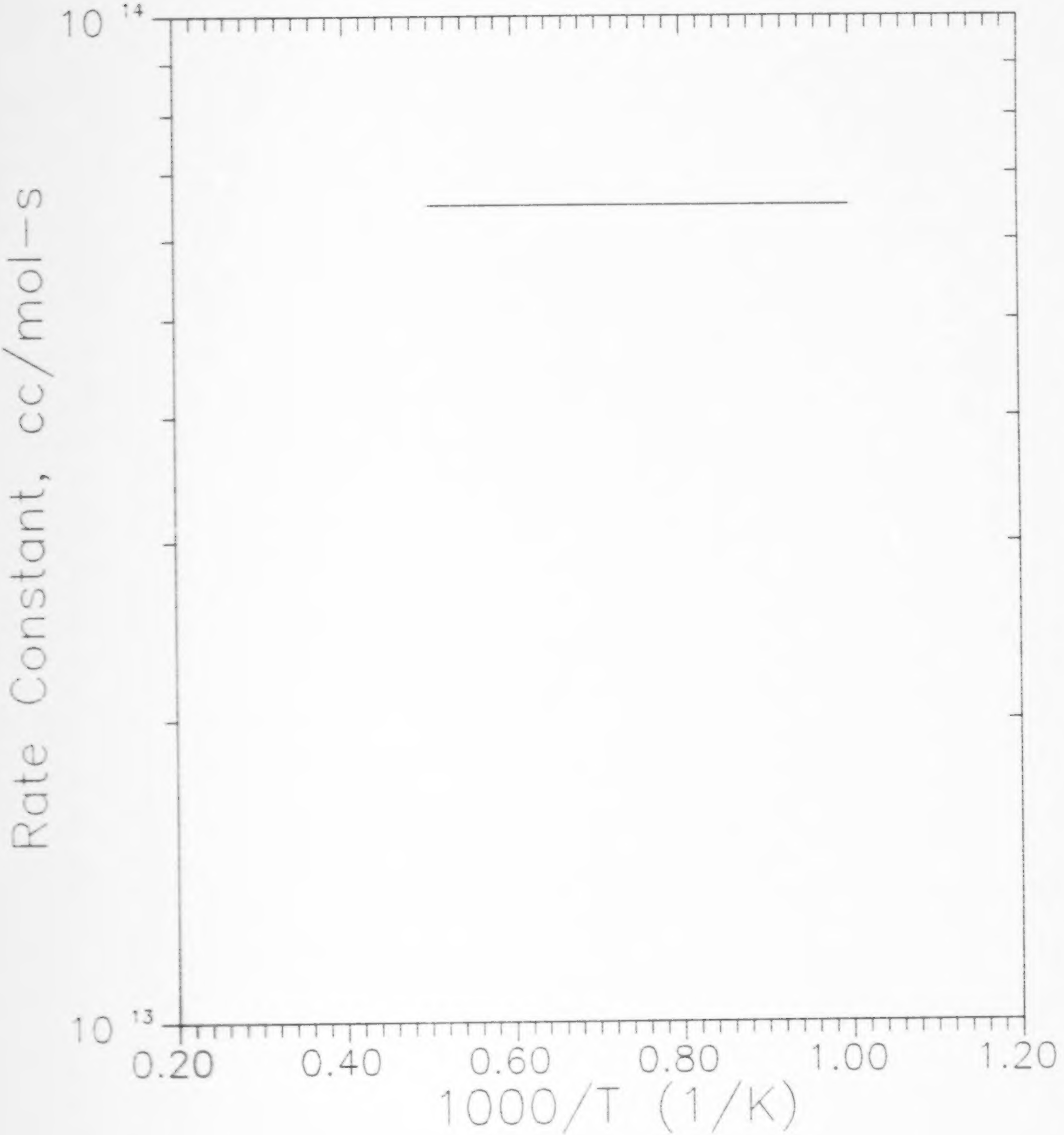
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O = CH + HO**



$10^{14}$
$10^{13}$
Rate Constant, cc/mol-s
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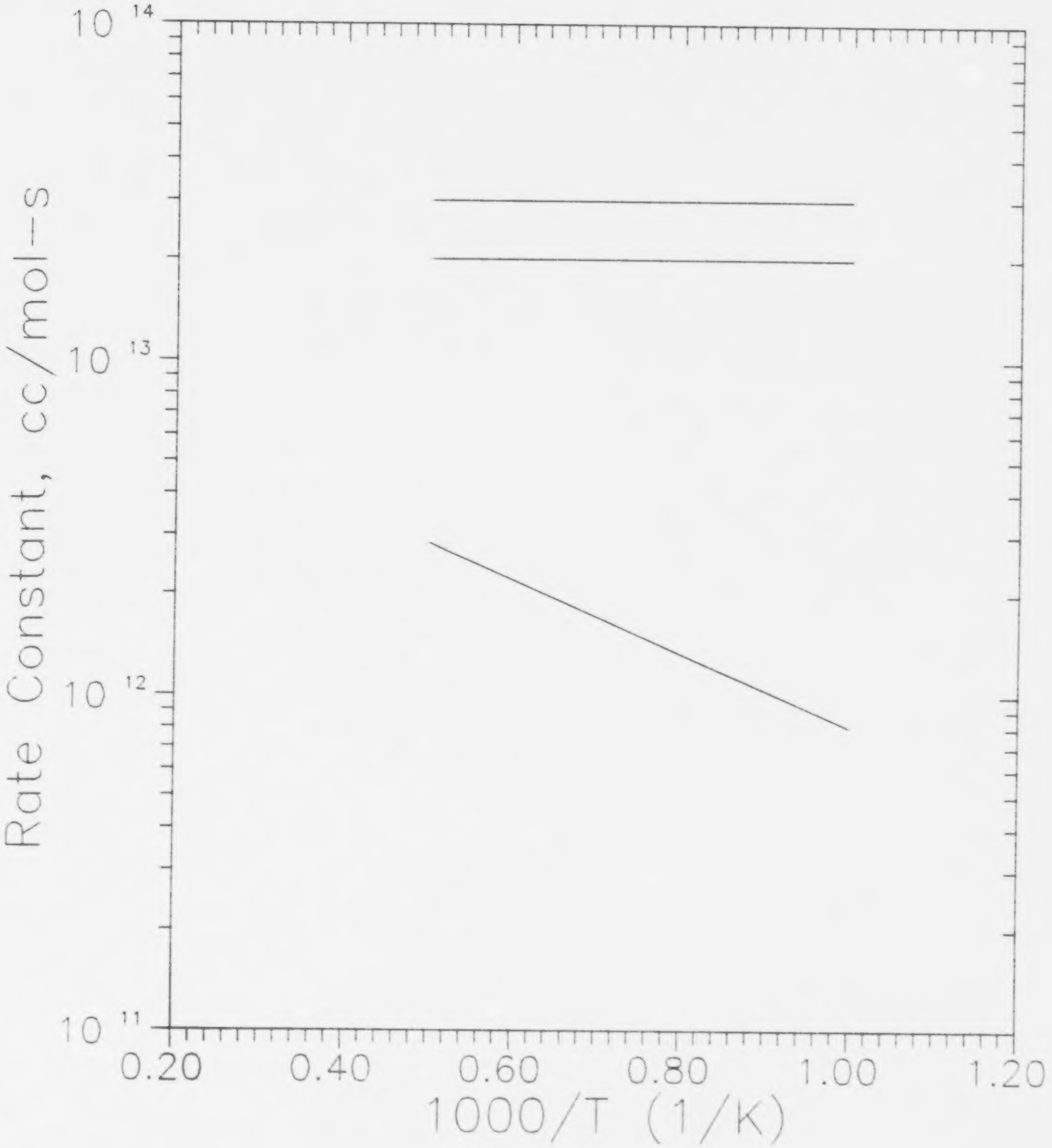
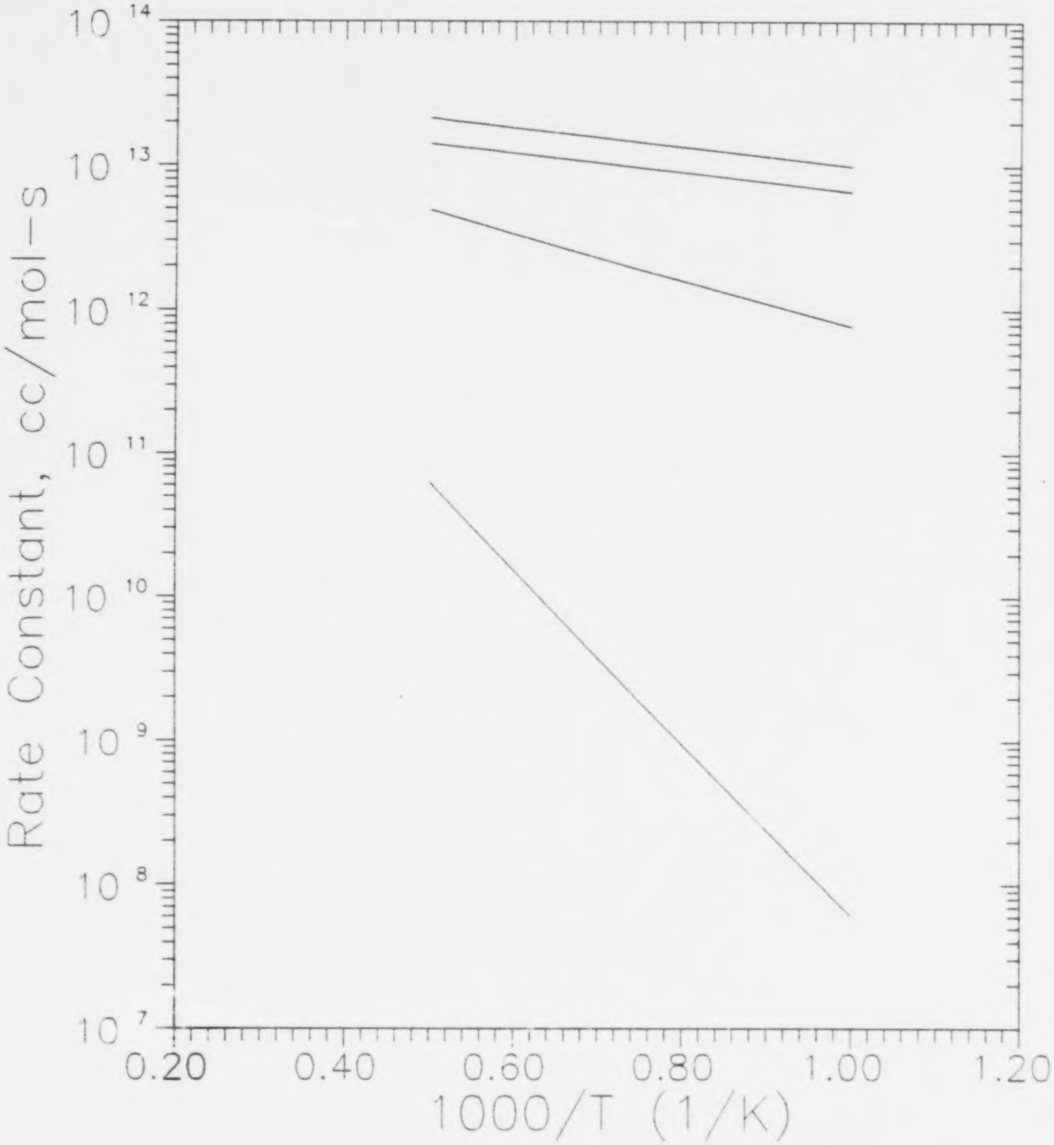
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + O = CHO + H**



Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + HO = CH2O + H**



Rate Constant, cc/mol-s
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10 12
10 11
10 10
10 9
10 8
10 7
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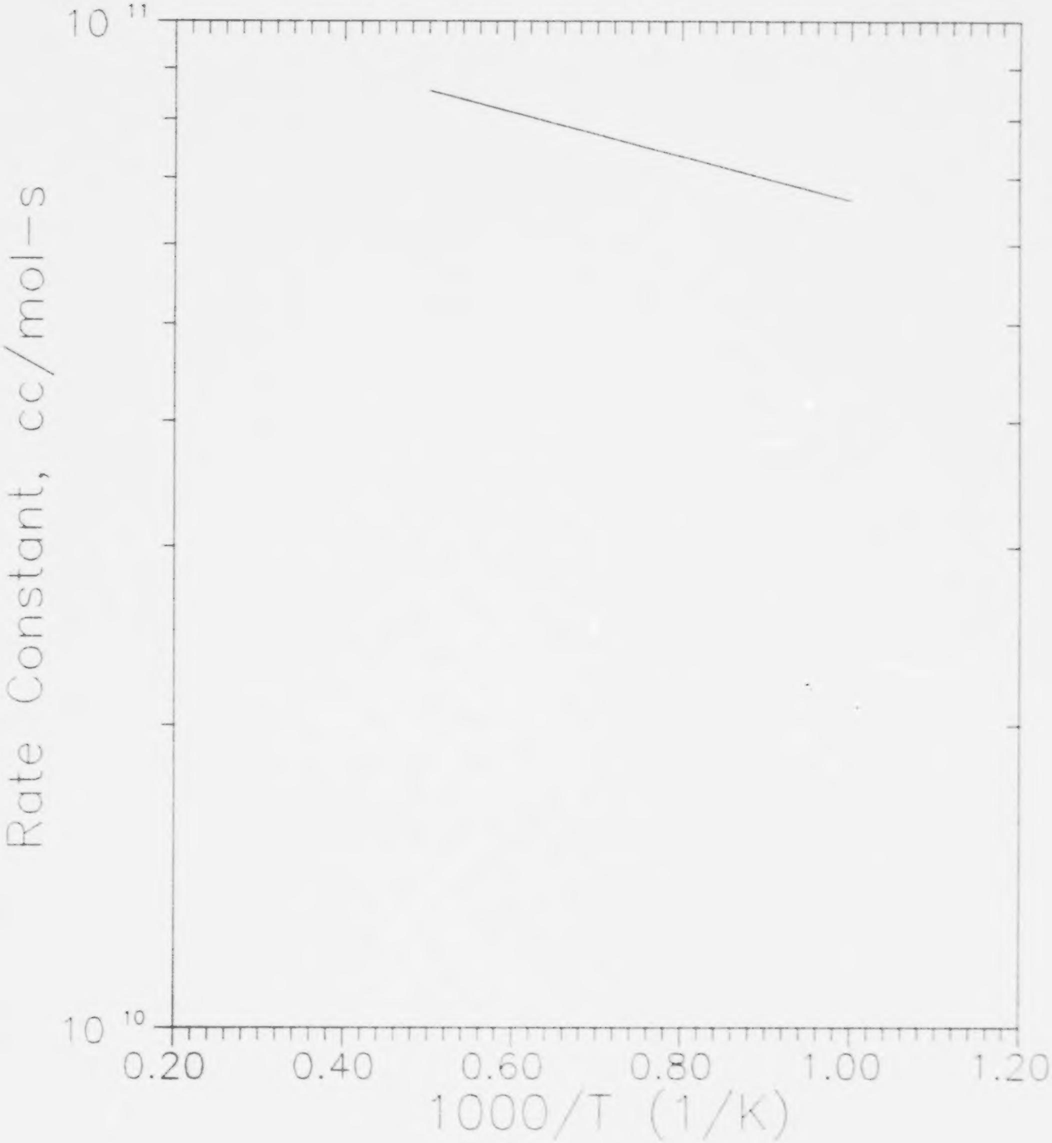
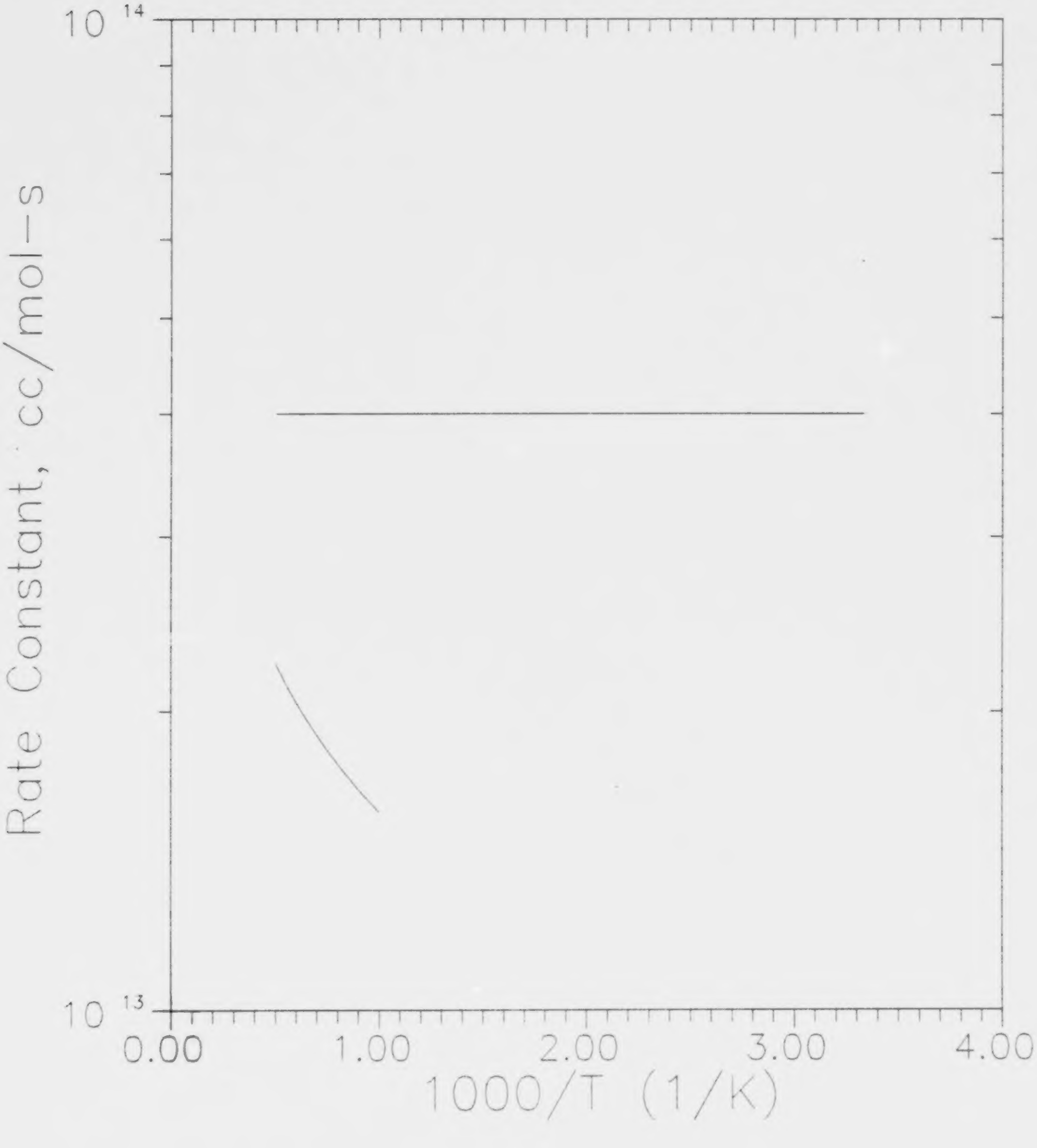
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

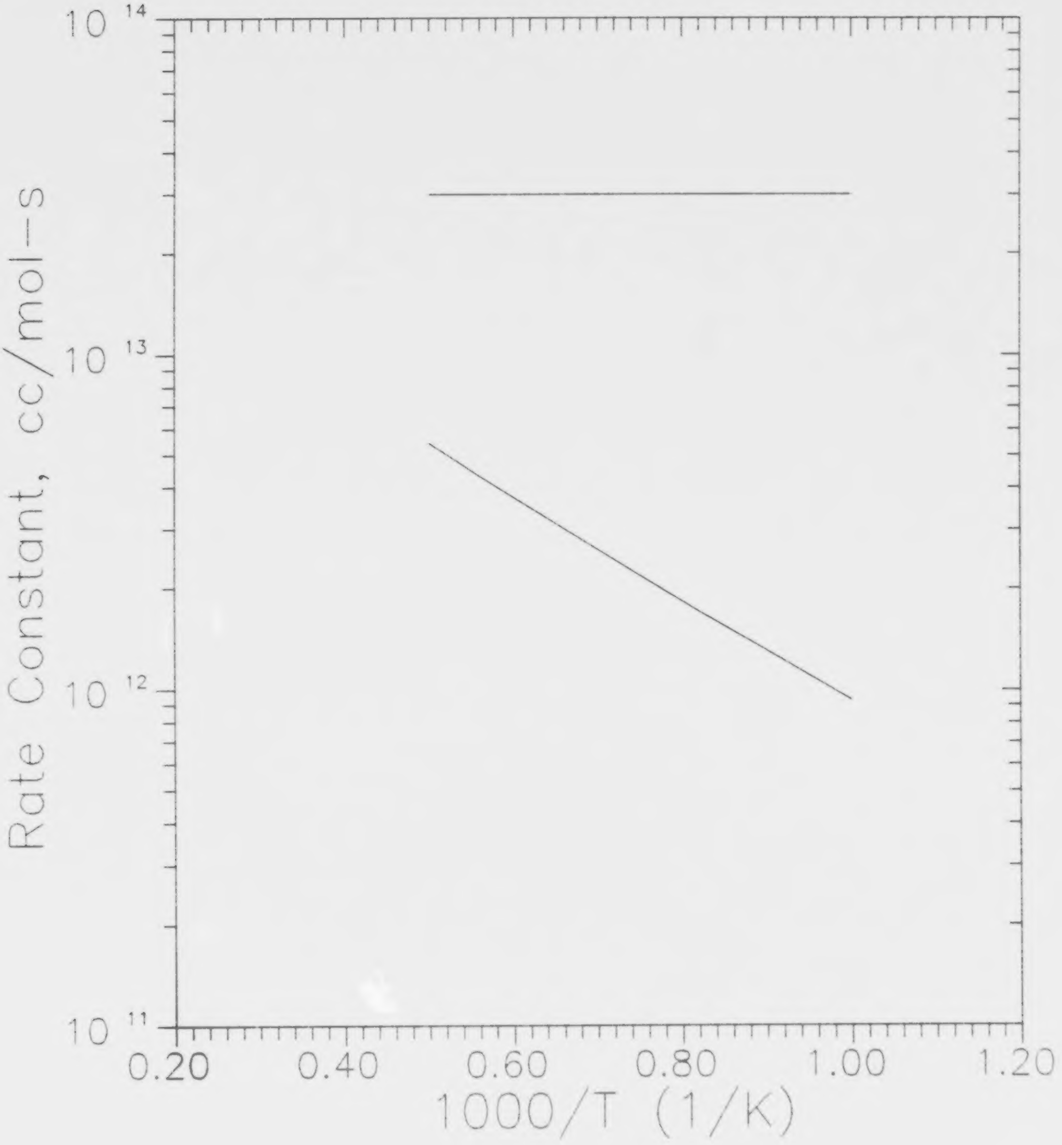
**CH2 + HO = CH + H2O**



**CH2 + CO2 = CO + CH2O**

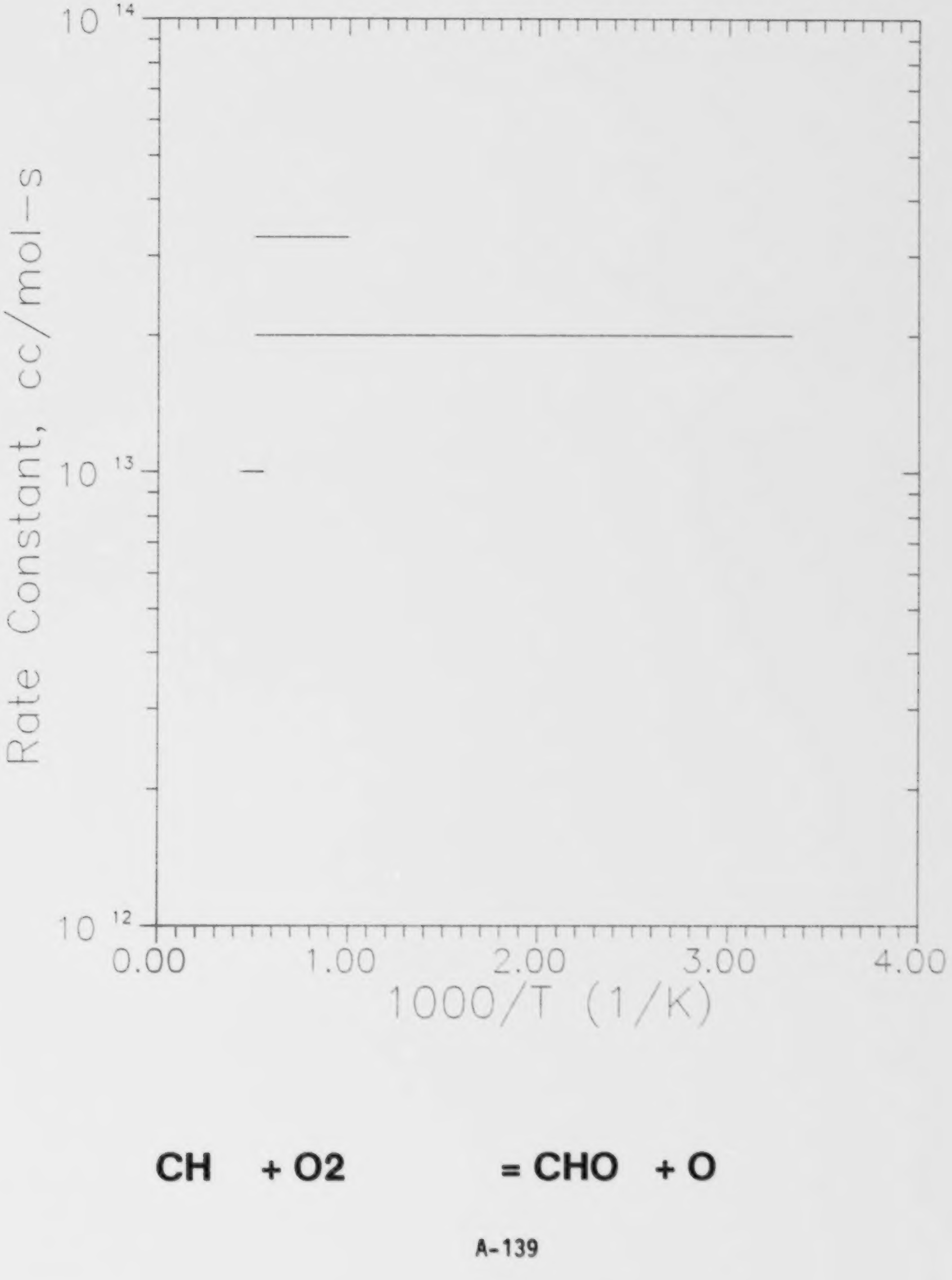


**CH + O = CO + H**



10 14
10 13
10 12
10 11
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH + HO = CHO + H**



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10 13
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Rate Constant, cc/mol-s
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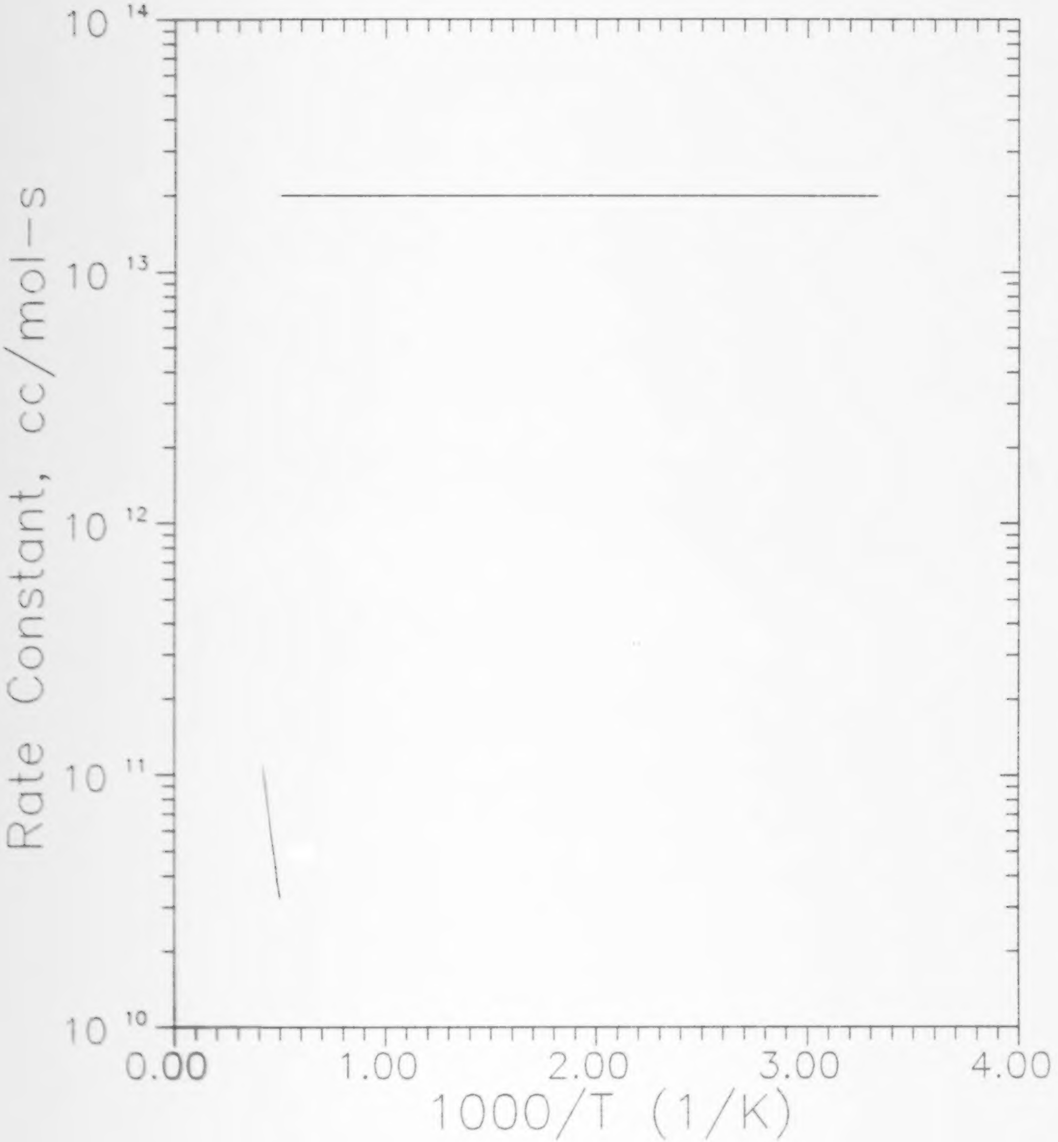
1.00
2.00
3.00
4.00
1000/T (1/K)

**CH + O2 = CHO + O**



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10 10
Rate Constant, cc/mol-s
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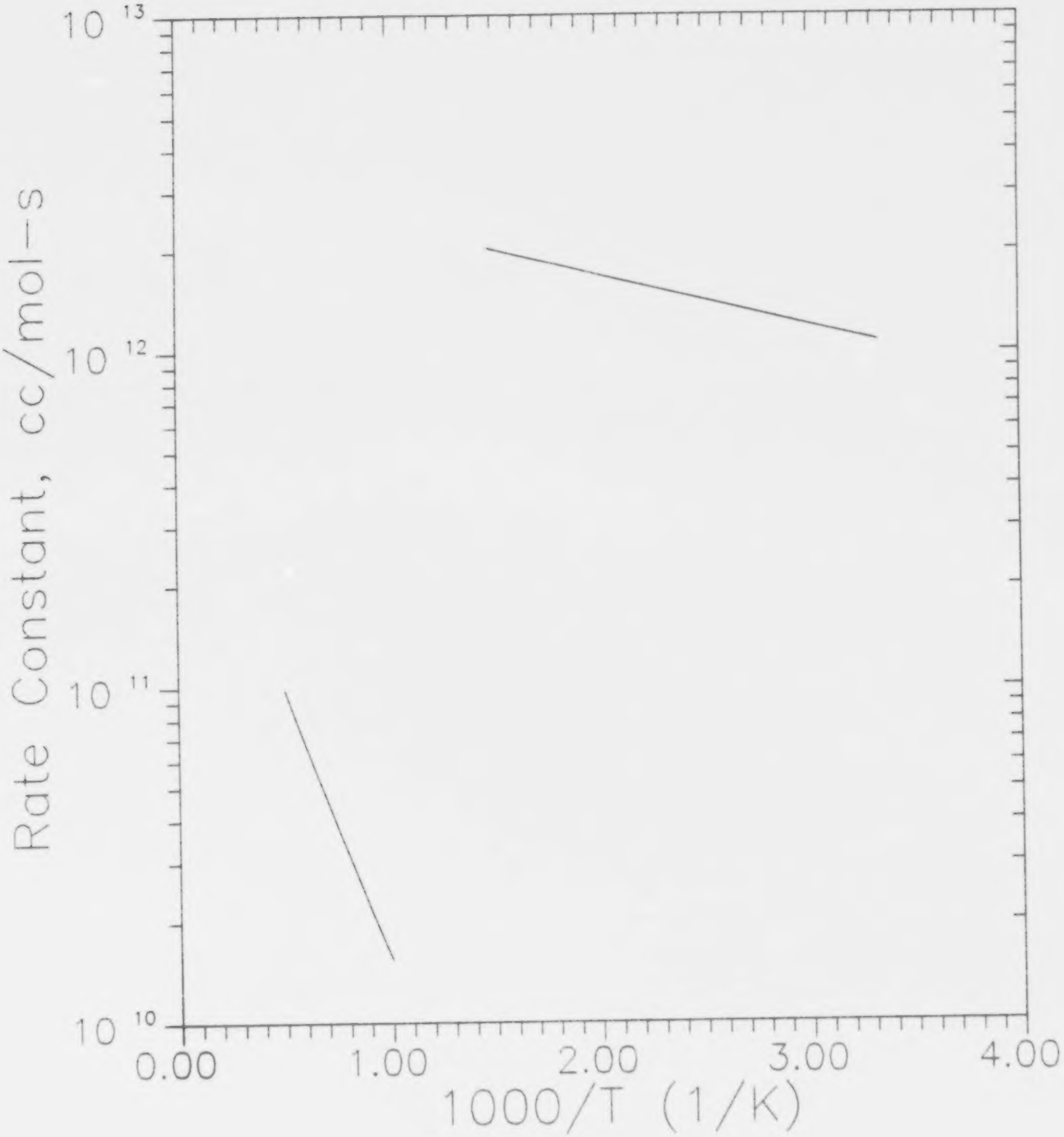
2.00
3.00
4.00
1000/T (1/K)

**CH + O2 = CO + HO**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10 12
10 11
10 10
Rate Constant, cc/mol-s
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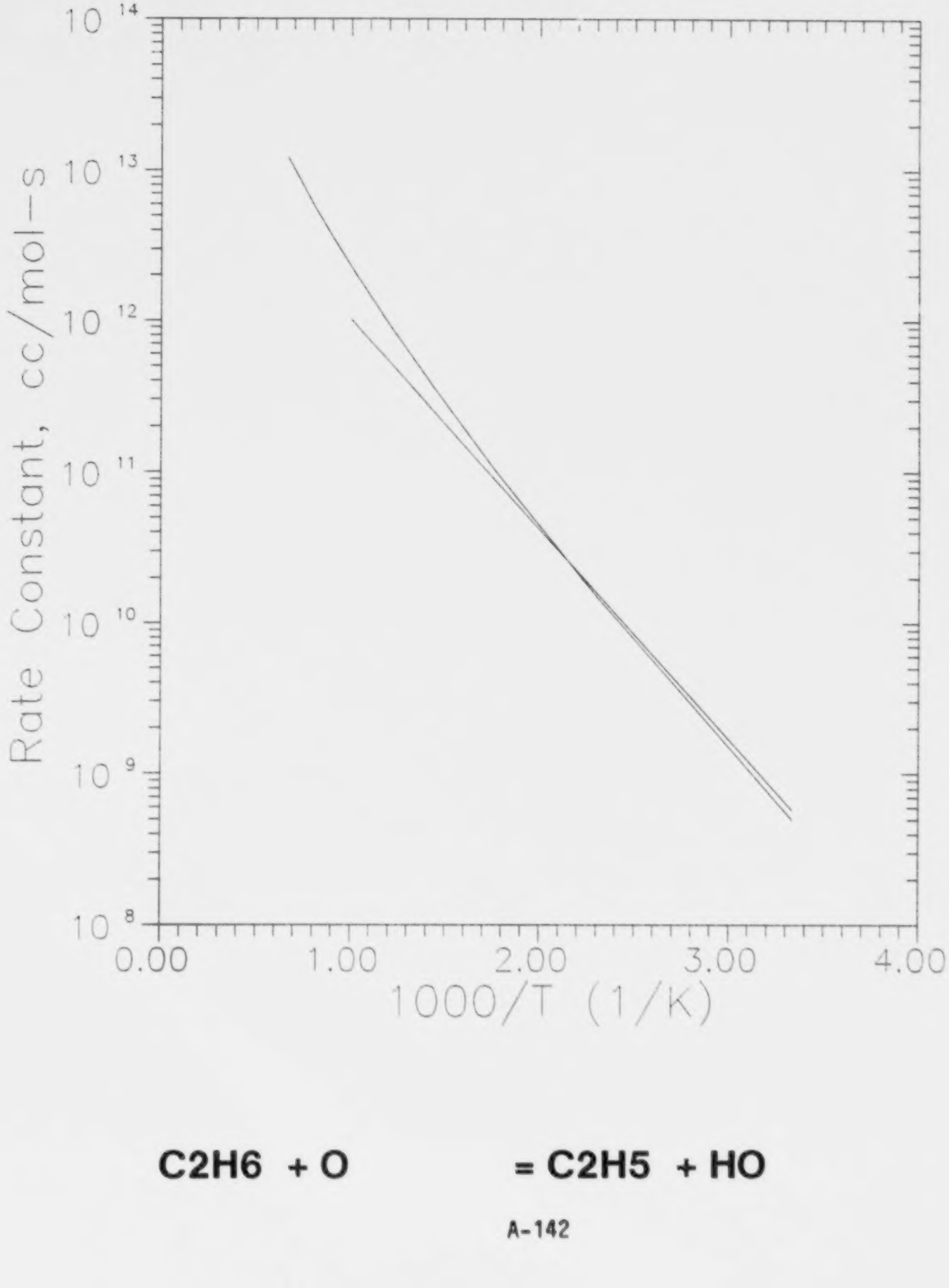
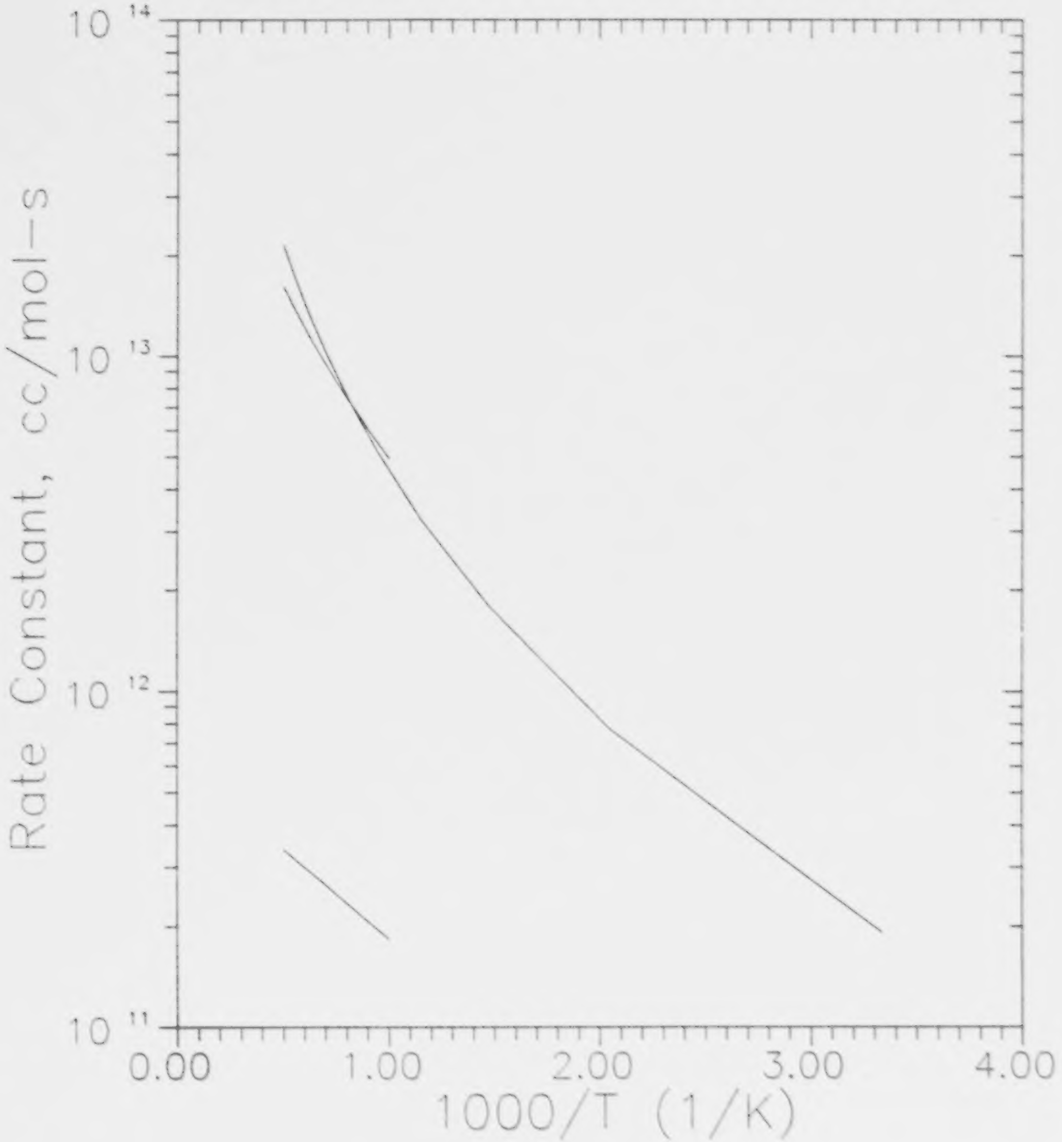
2.00
3.00
4.00
1000/T (1/K)

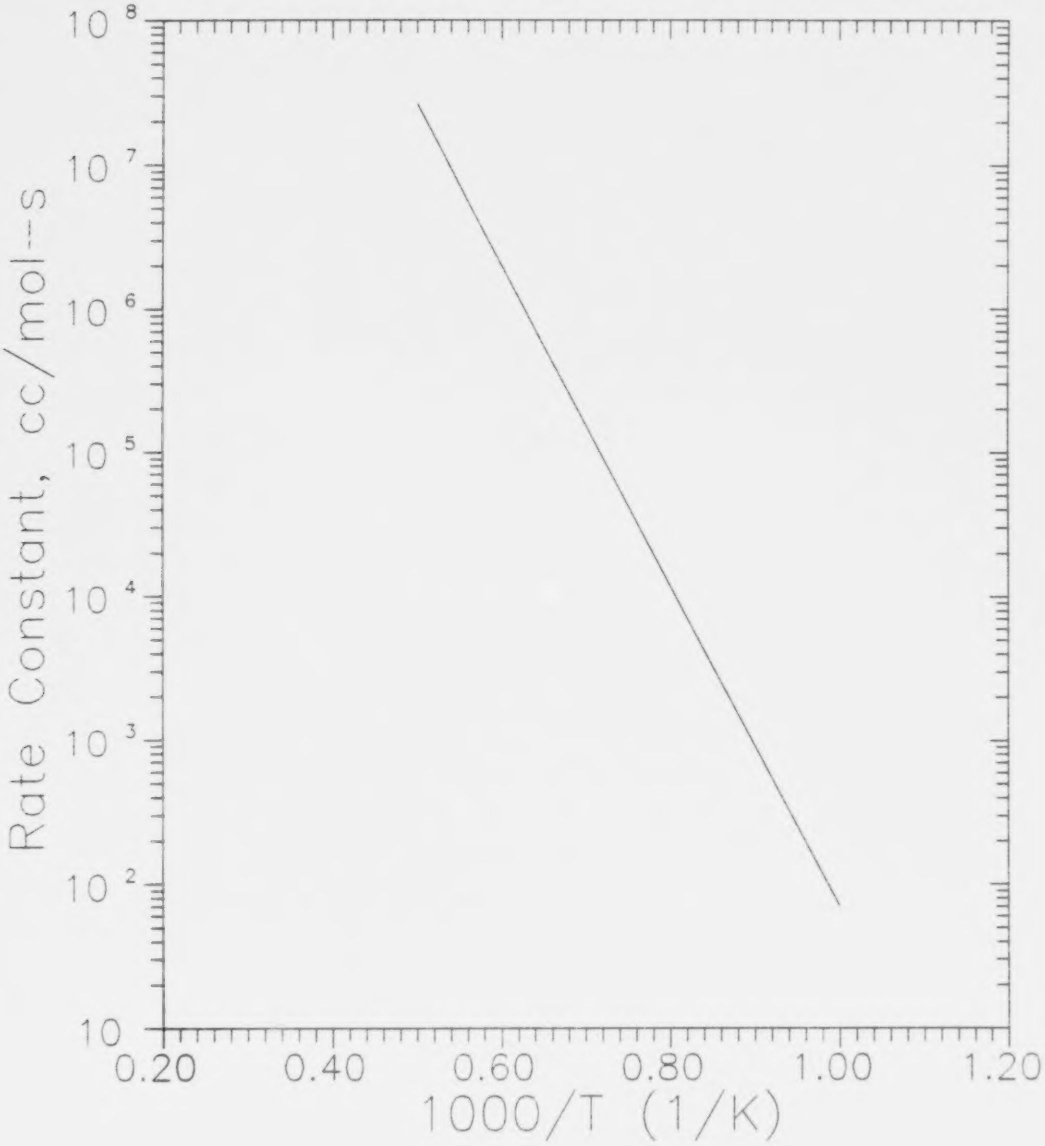
**CH + CO2 = CHO + CO**



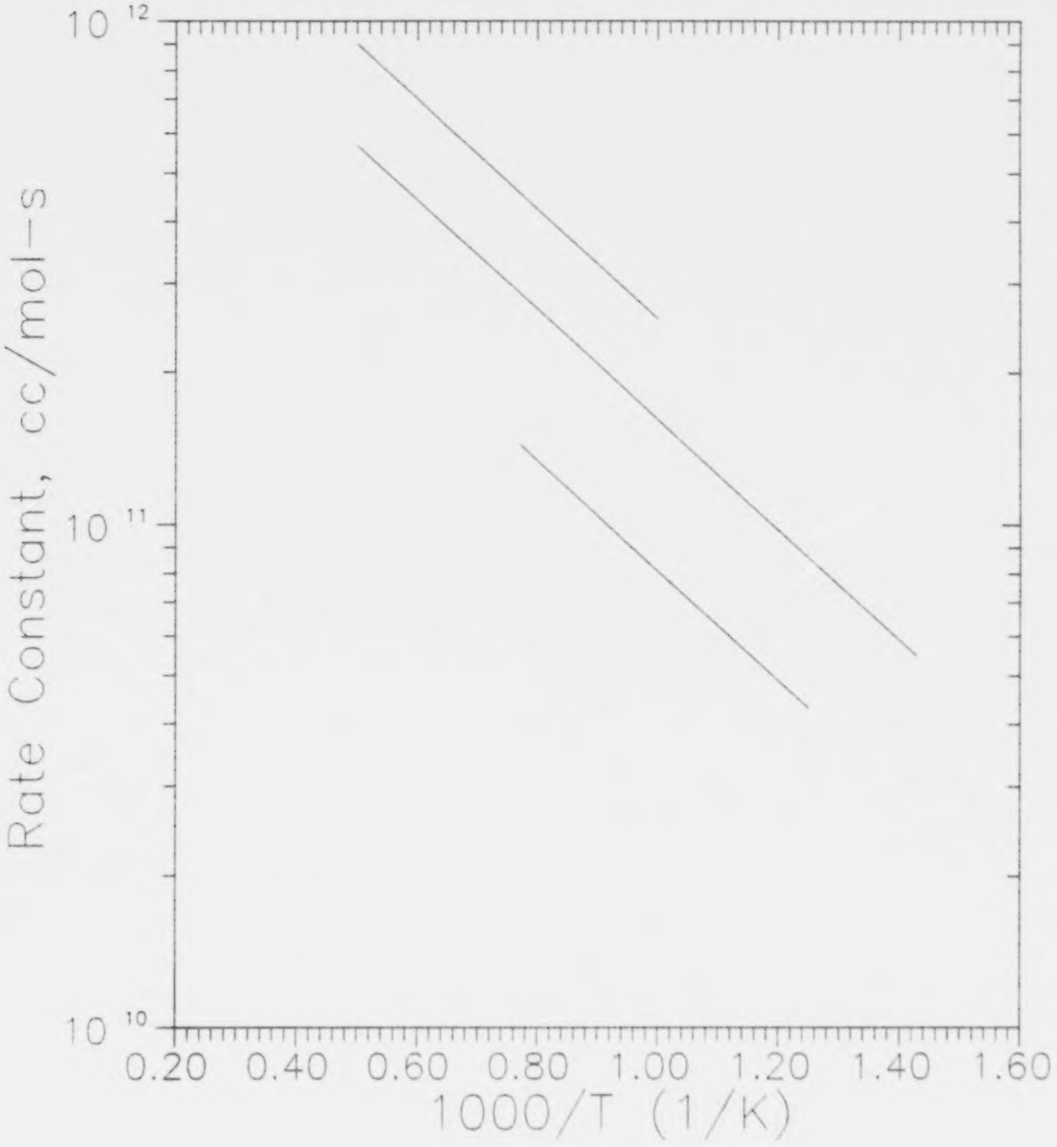
**C2H6 + O = C2H5 + HO**



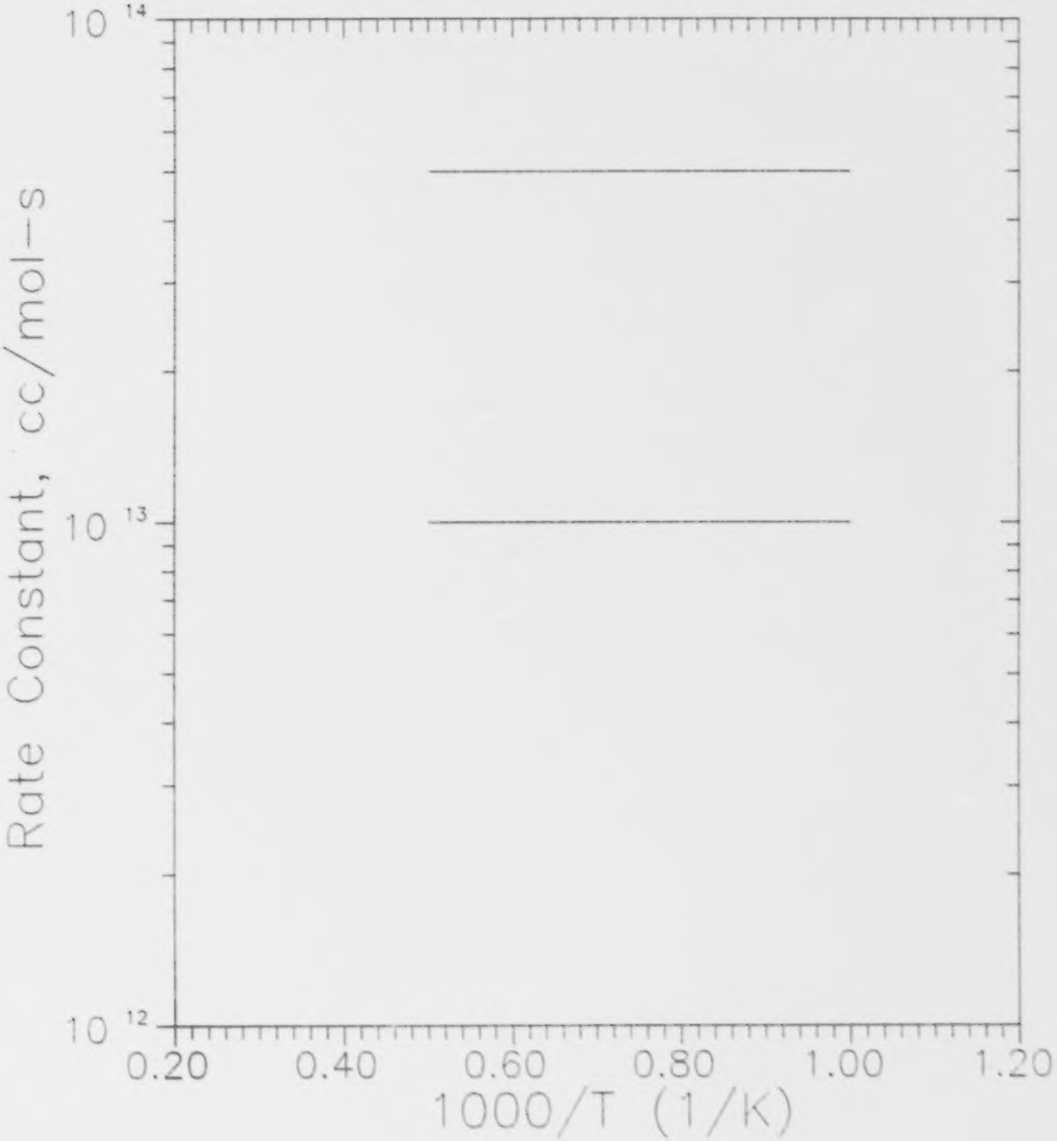
**C2H6 + HO = C2H5 + H2O**



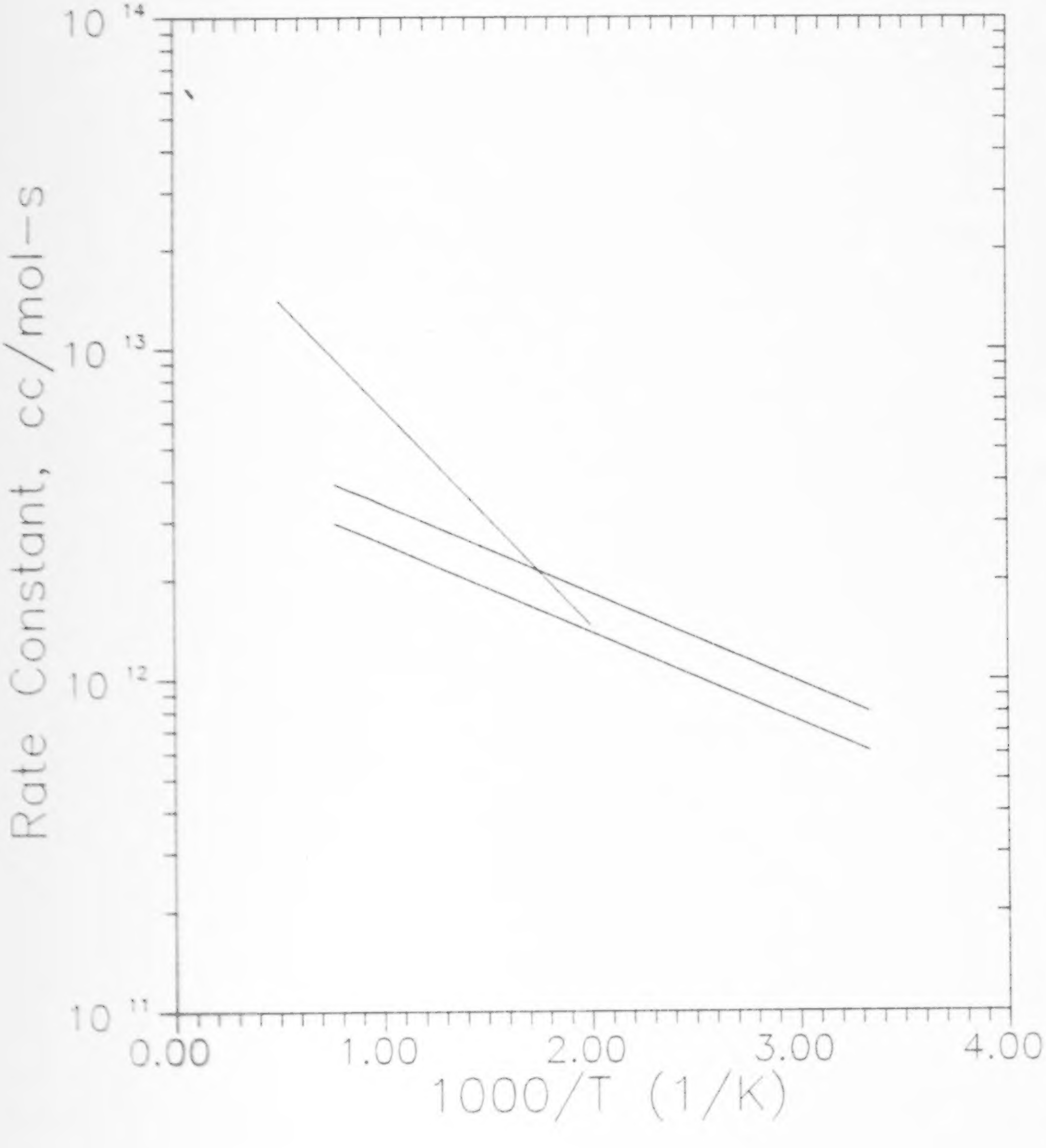
**C2H6 + O2 = C2H5 + HO2**



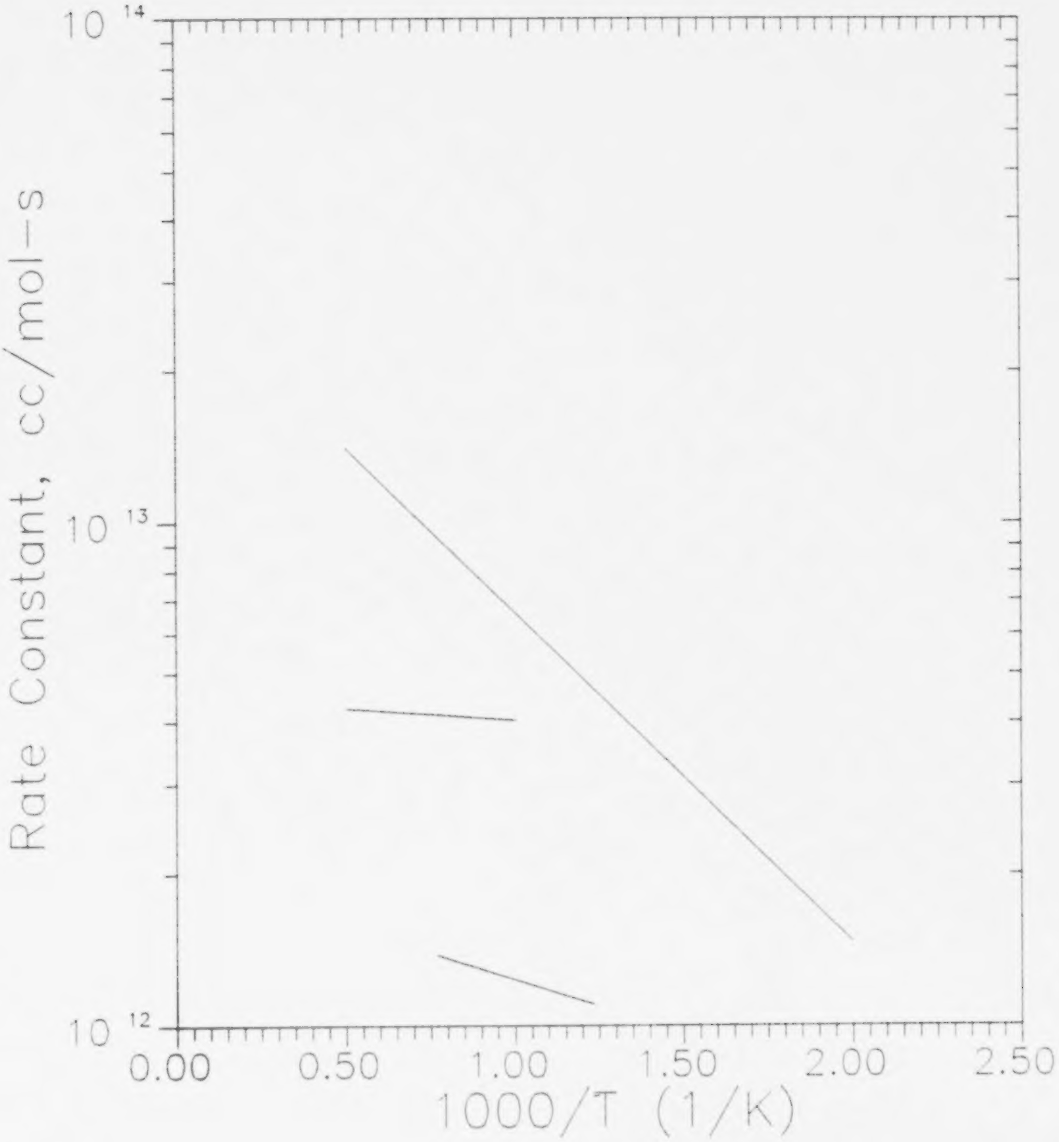
**C2H5 + O2 = C2H4 + HO2**



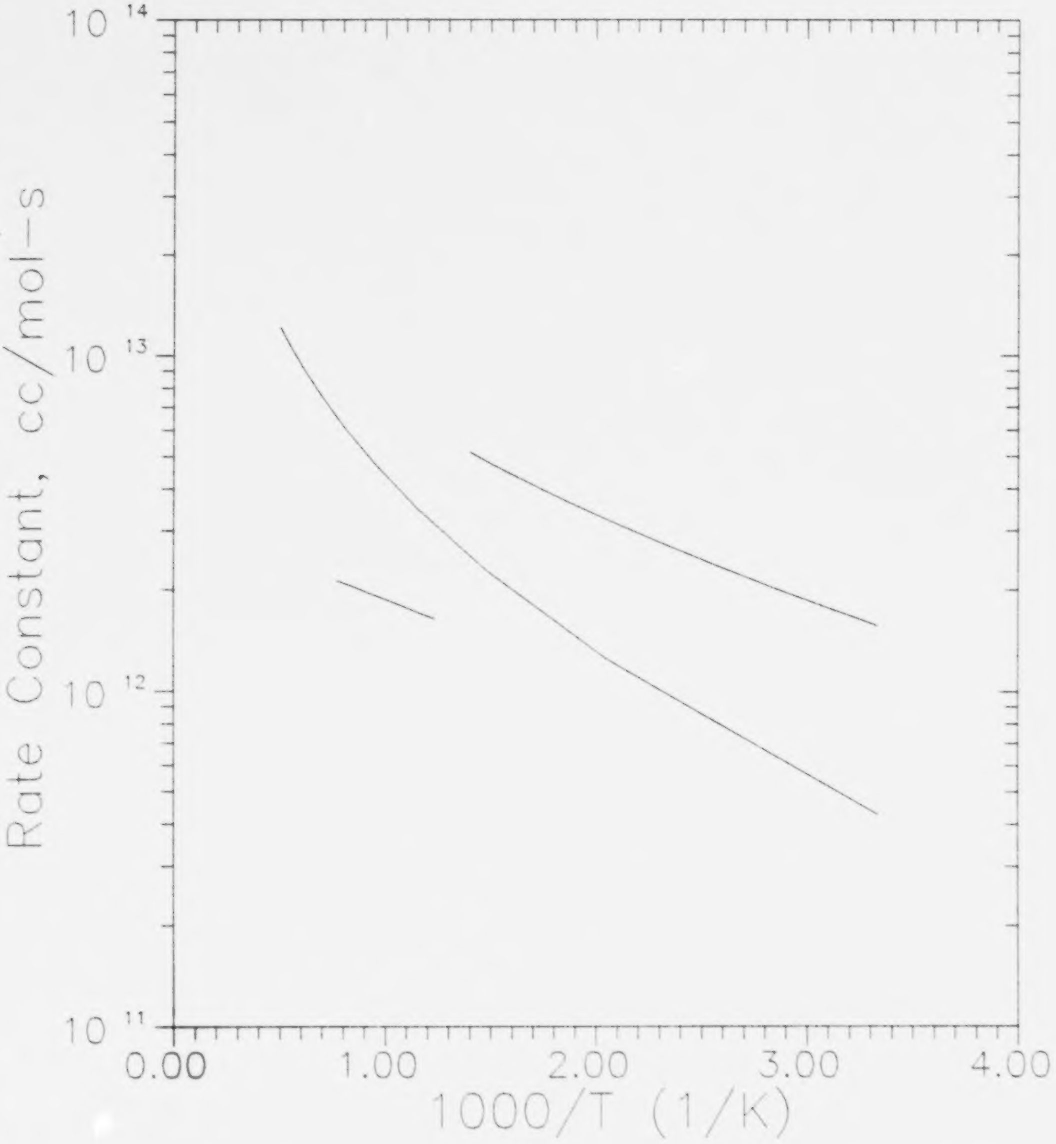
**C2H5 + O = CH2O + CH3**



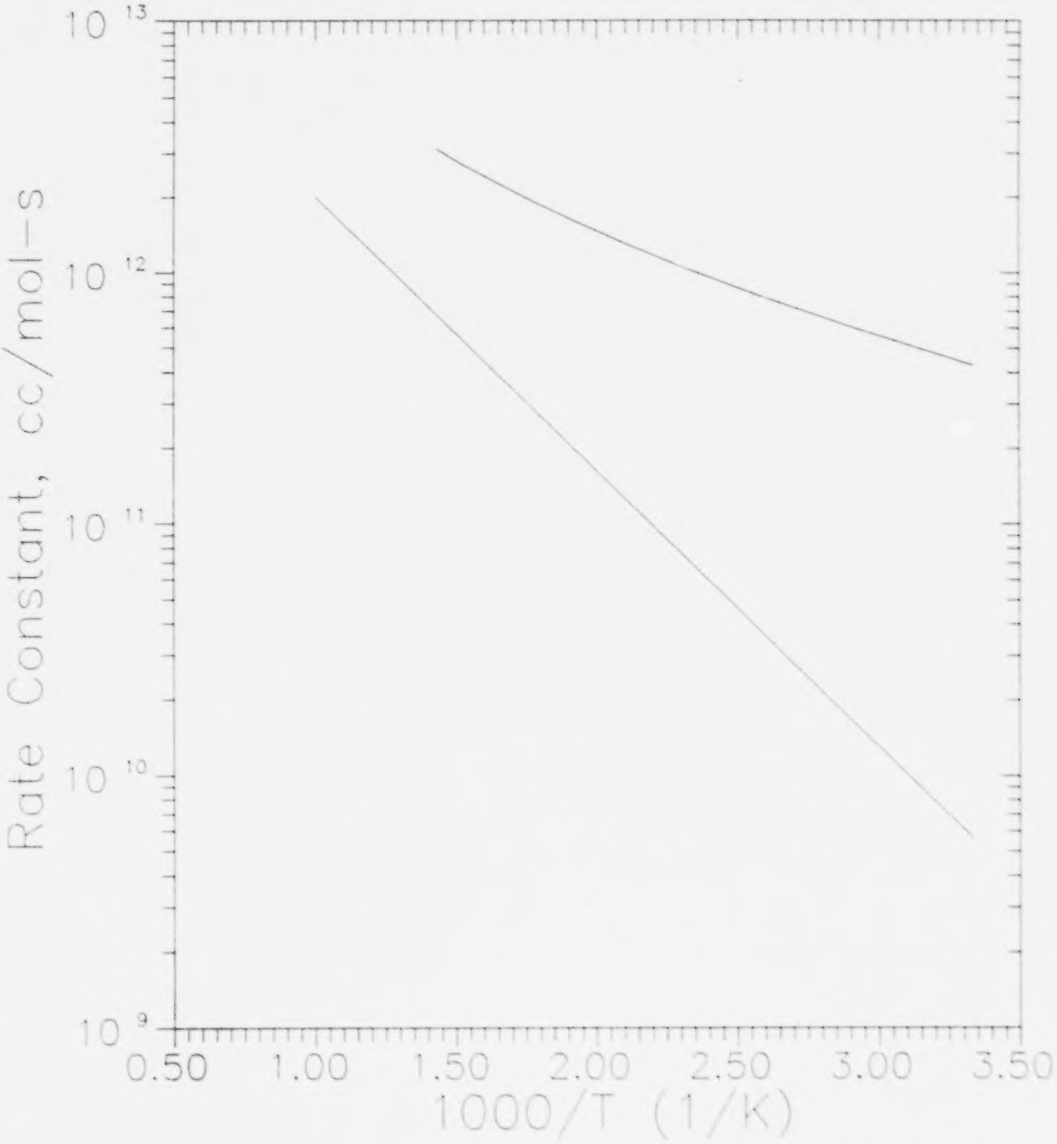
**C2H4 + HO = C2H3 + H2O**



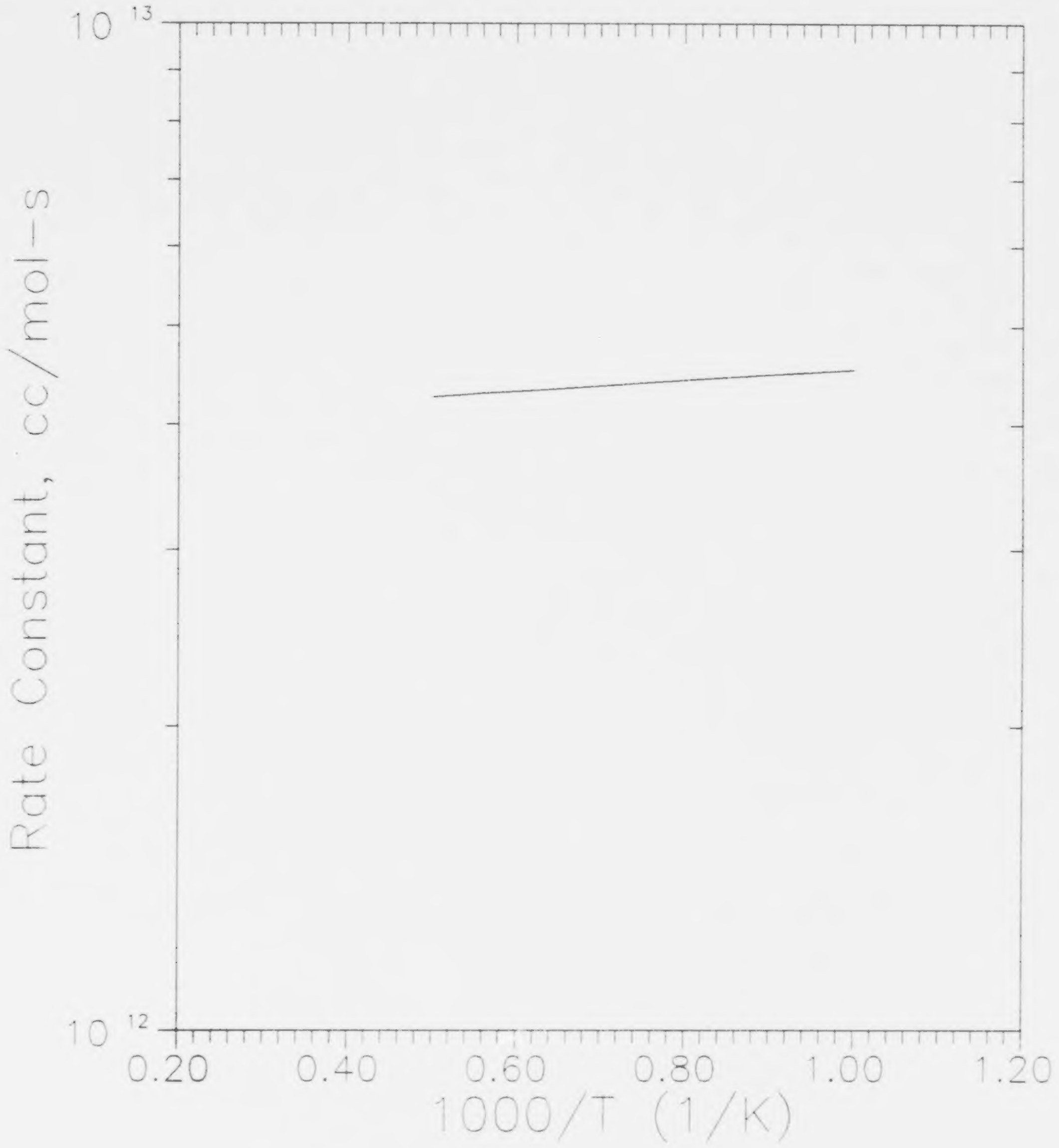
**C2H4 + HO = CH2O + CH3**



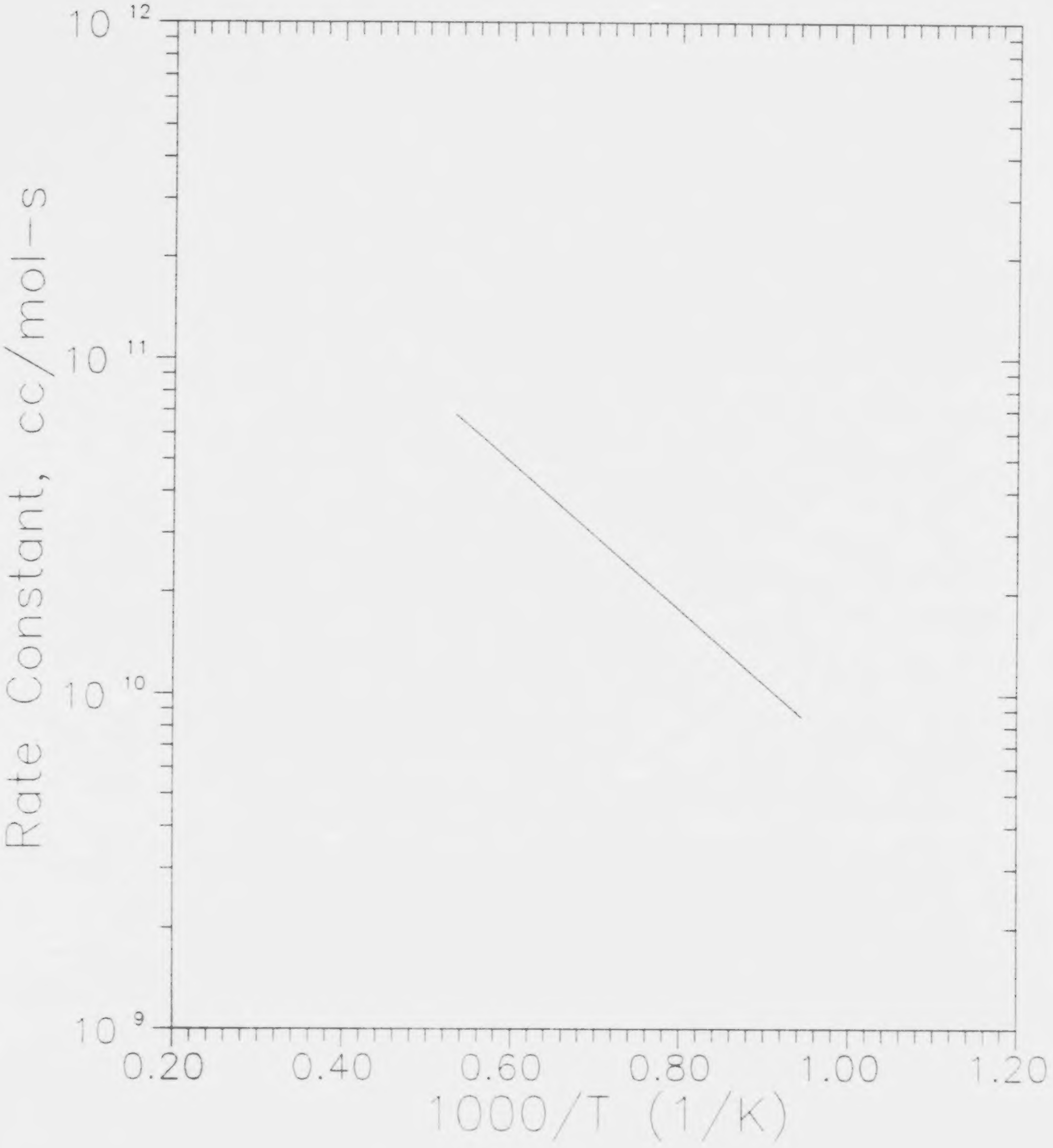
C2H4 + O = CHO + CH3



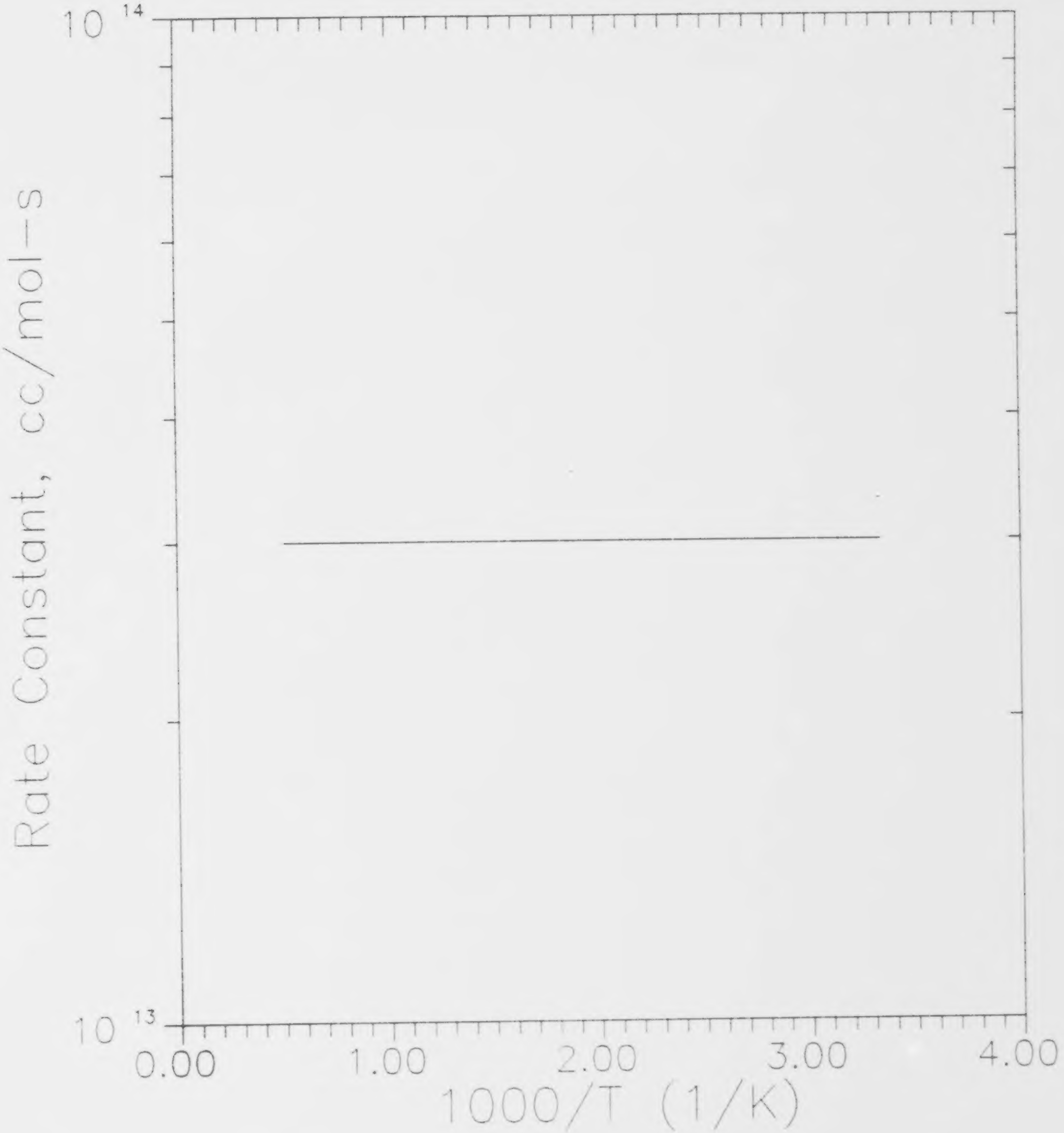
**C2H4 + O = CH2O + CH2**



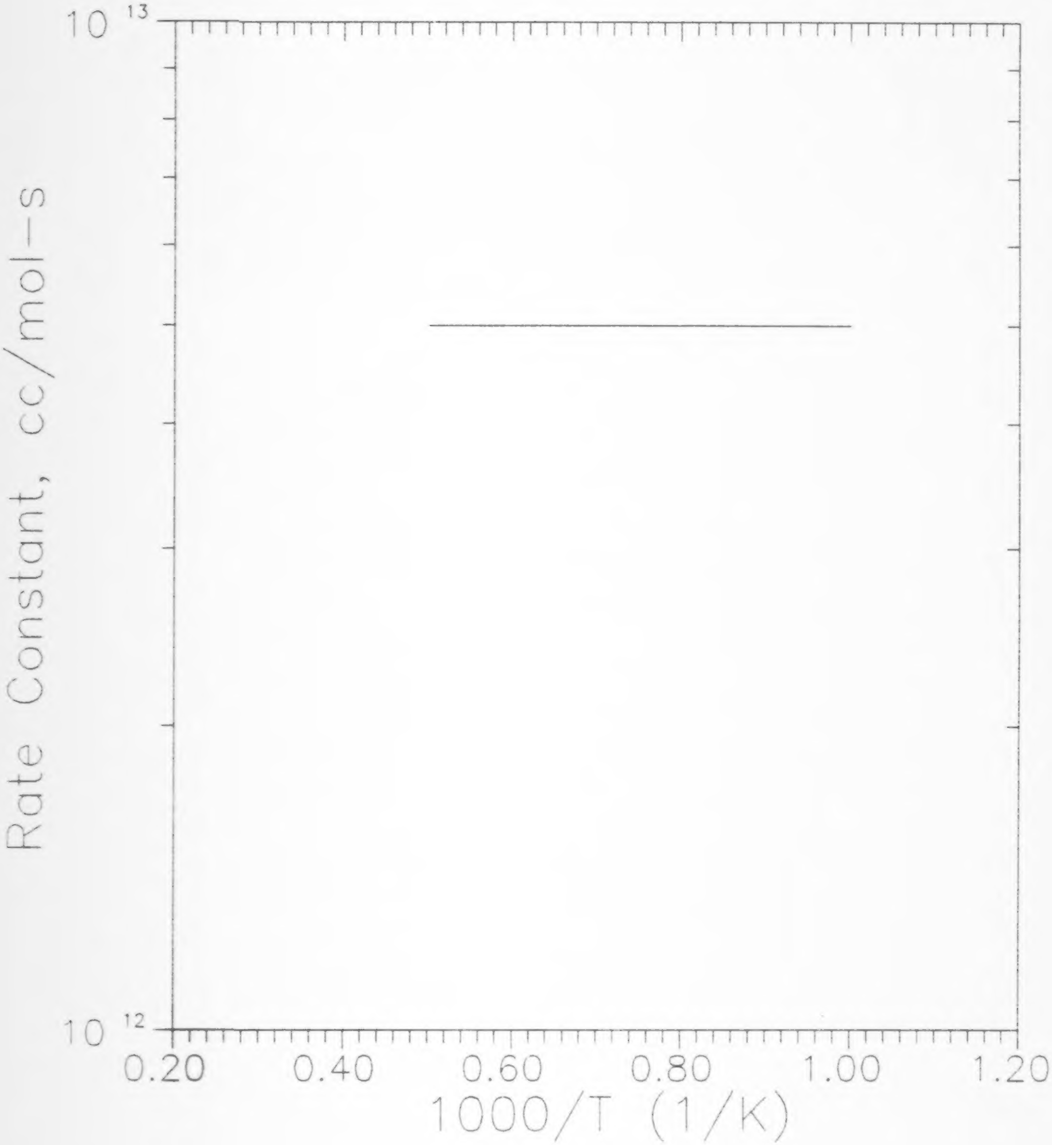
**C2H3 + O2 = CHO + CH2O**



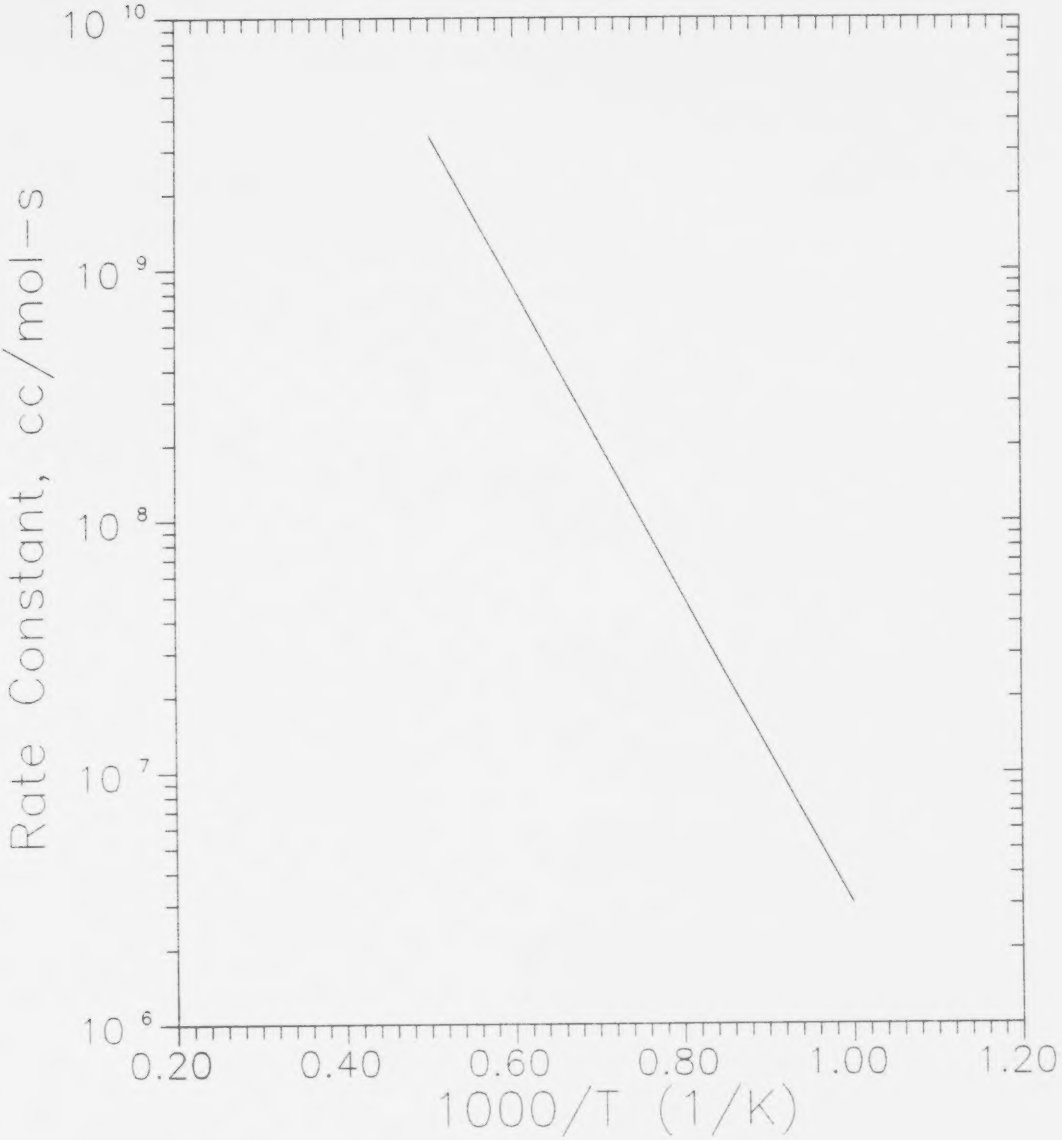
**$C_2H_3$ + $O_2$ = $C_2H_2$ + $HO_2$**



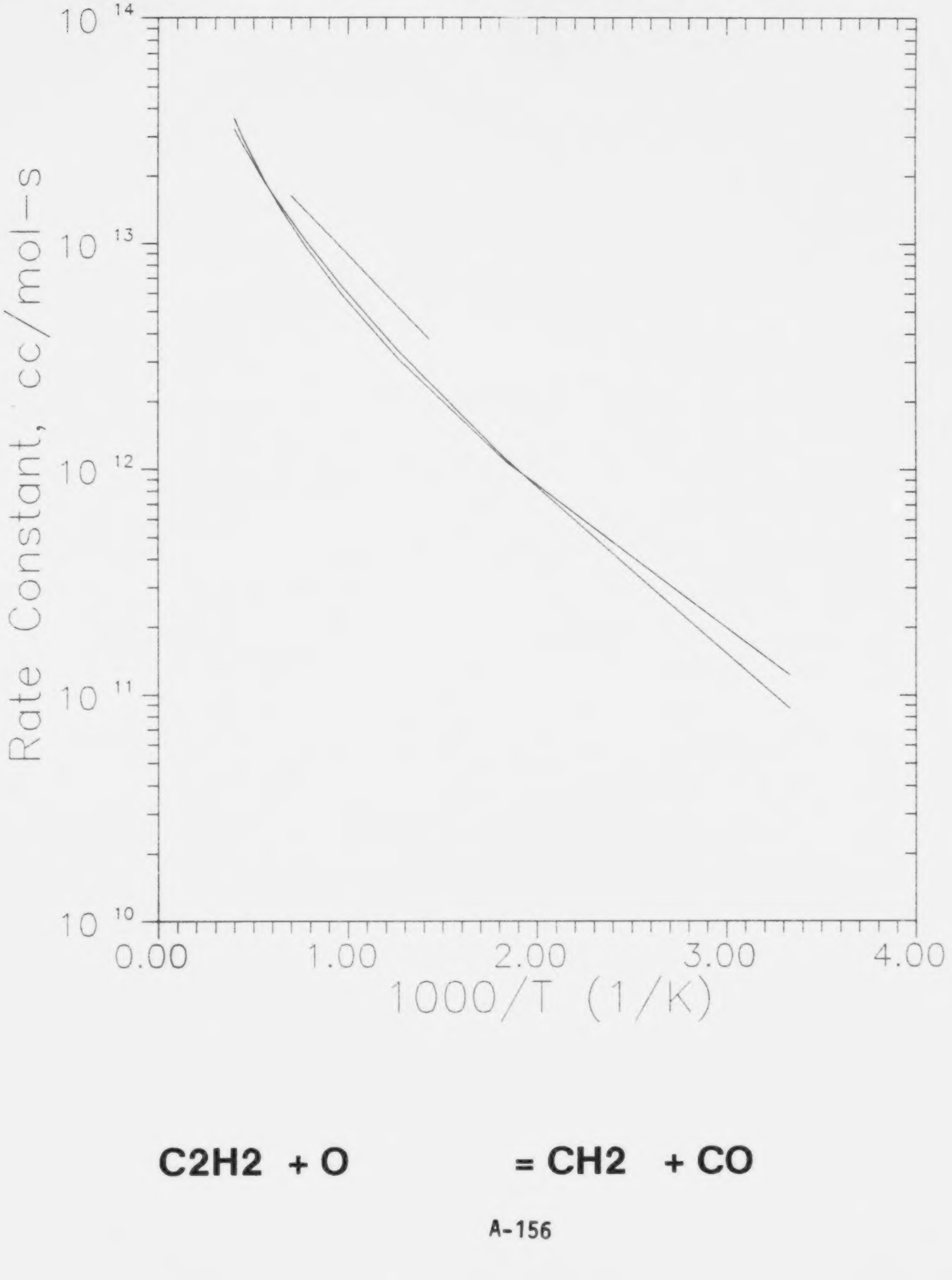
**C2H3 + O = CH2CO + H**



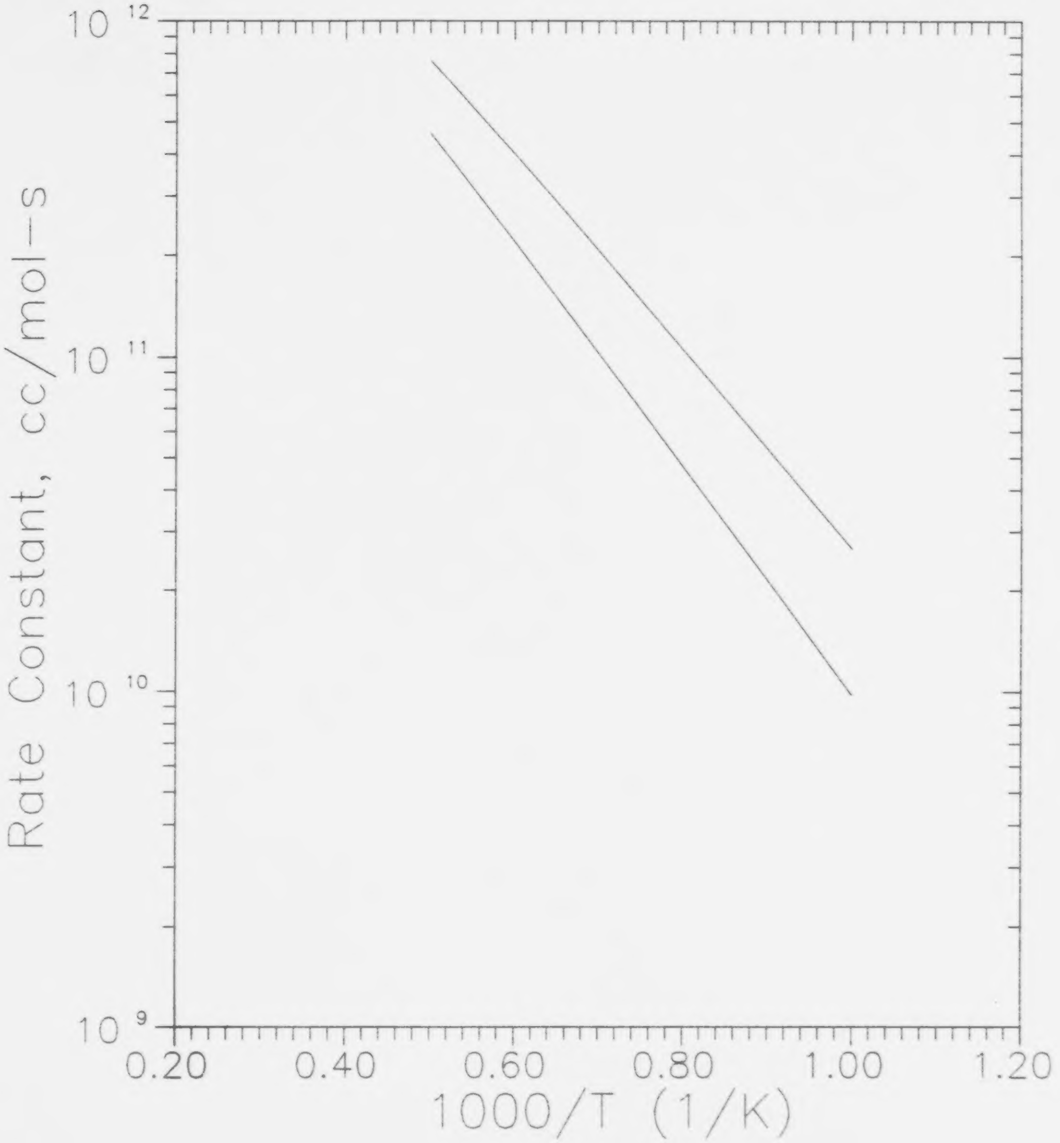
**C2H3 + HO = C2H2 + H2O**



**C2H2 + O2 = CHO + CHO**

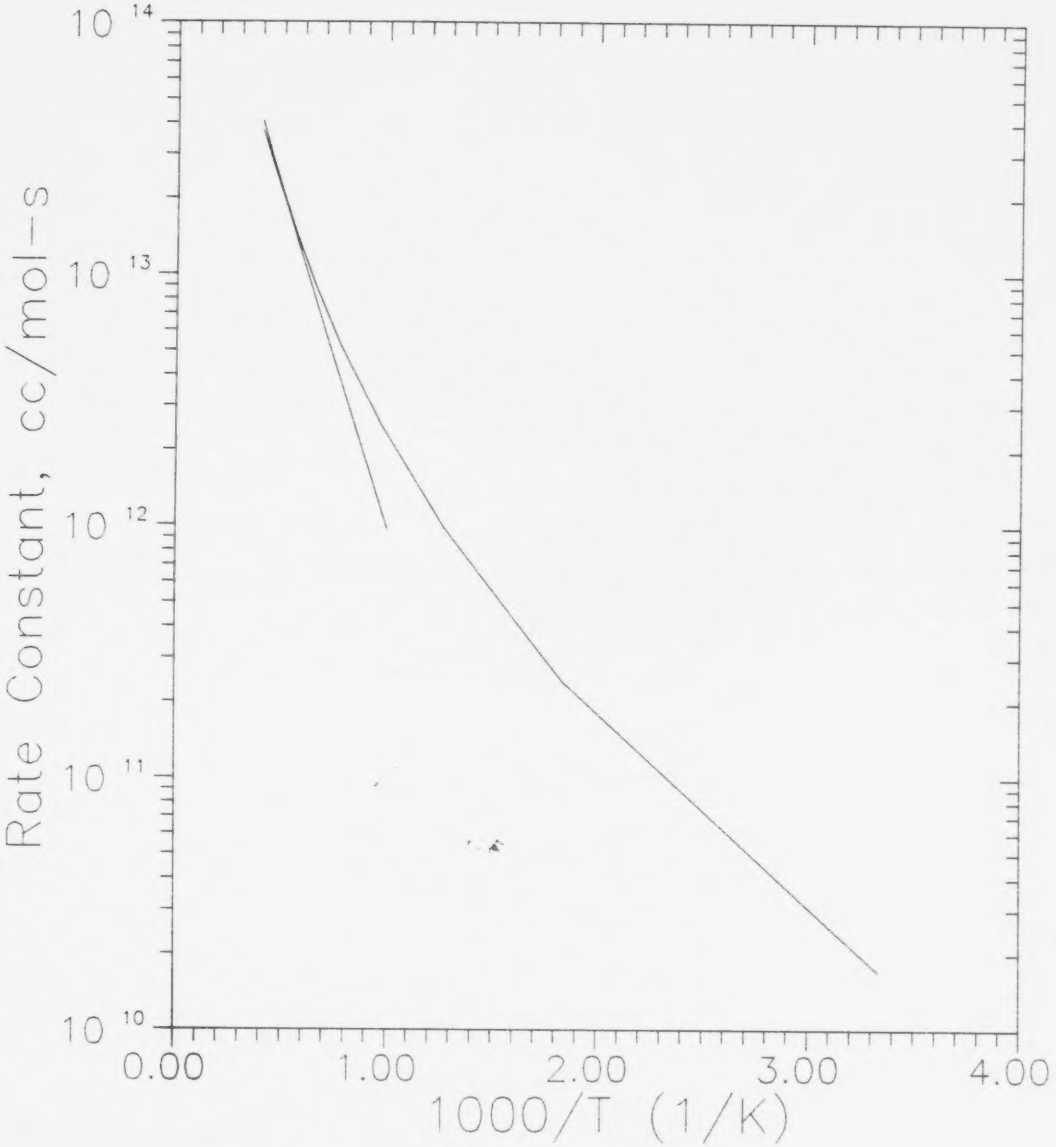

Rate Constant, cc/mol-s
10^14
10^13
10^12
10^11
10^10
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**C2H2 + O = CH2 + CO**



10 12
10 11
10 10
10 9
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**$C_2H_2$ + O = $C_2H$ + HO**


Rate Constant, cc/mol-s
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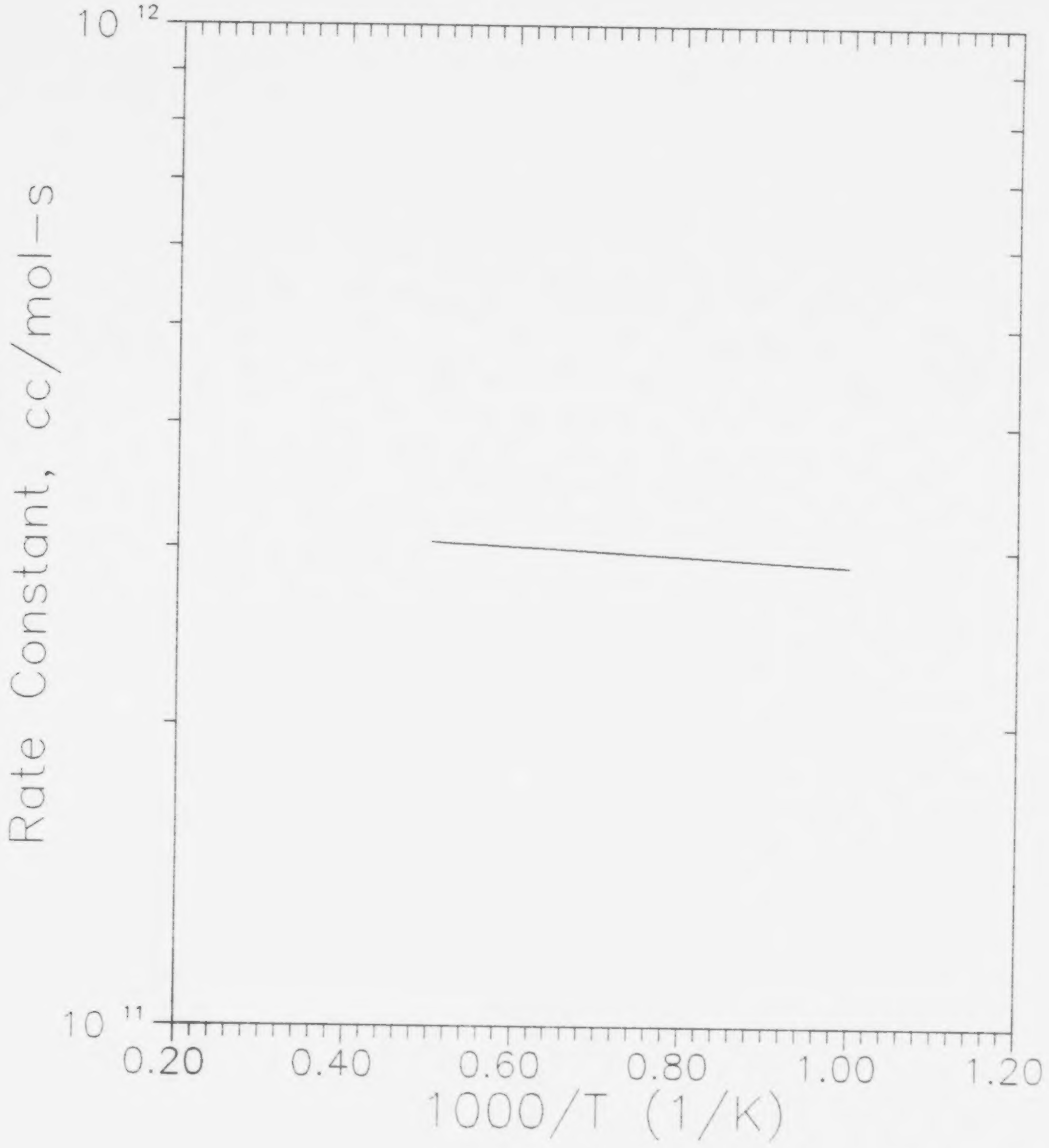
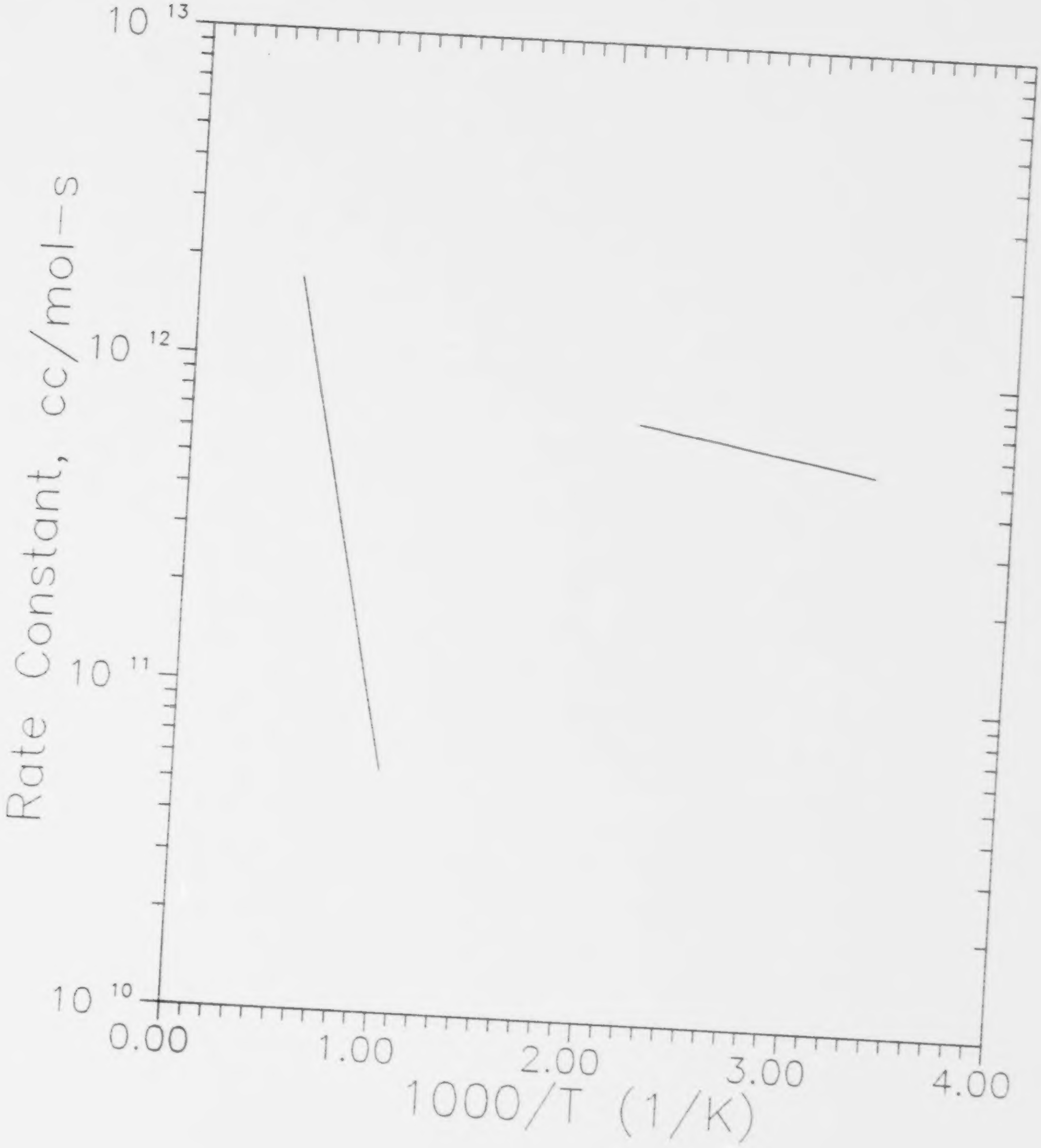
$10^{13}$
$10^{12}$
$10^{11}$
$10^{10}$
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

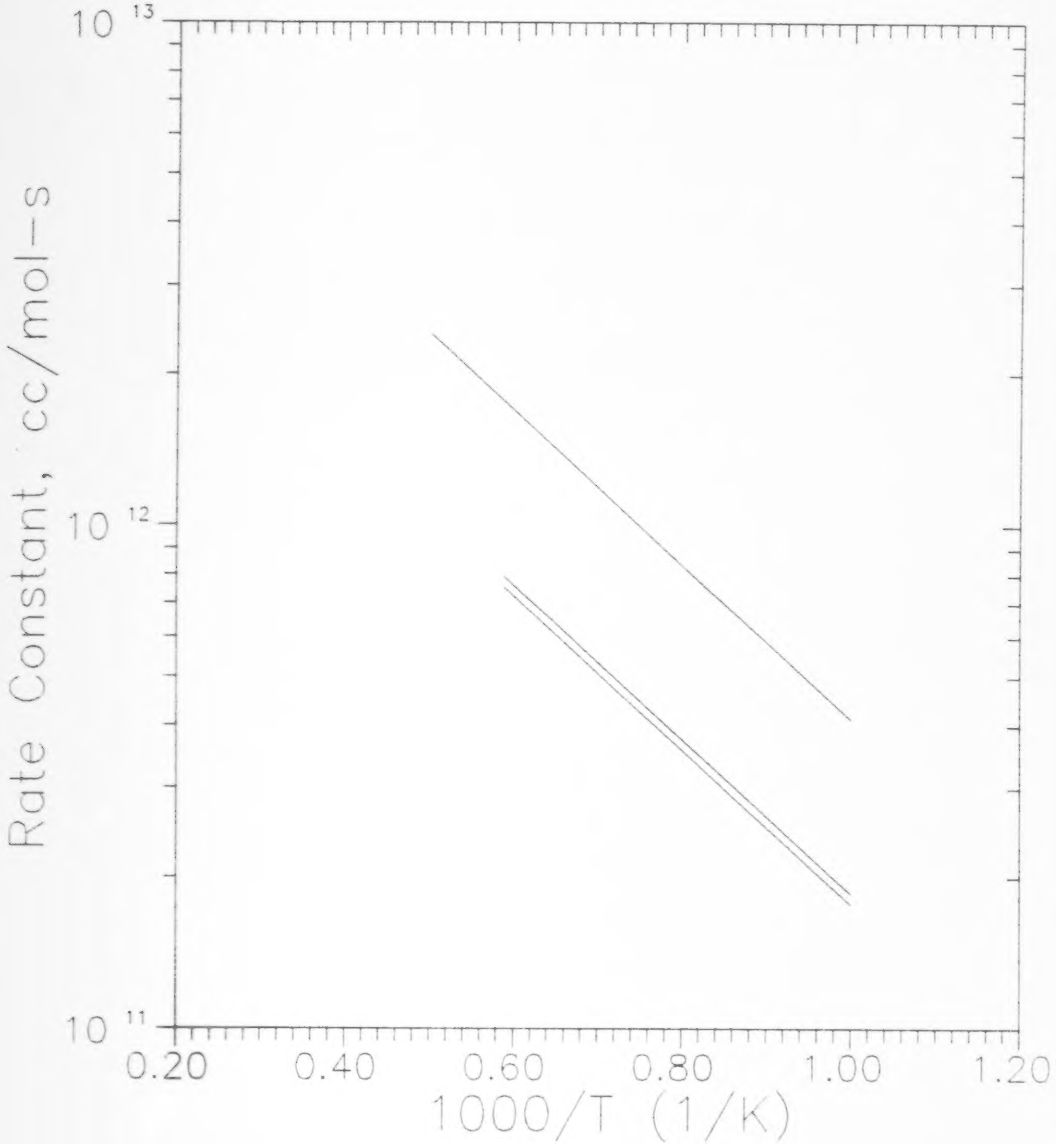
**C2H2 + O = CHCO + H**



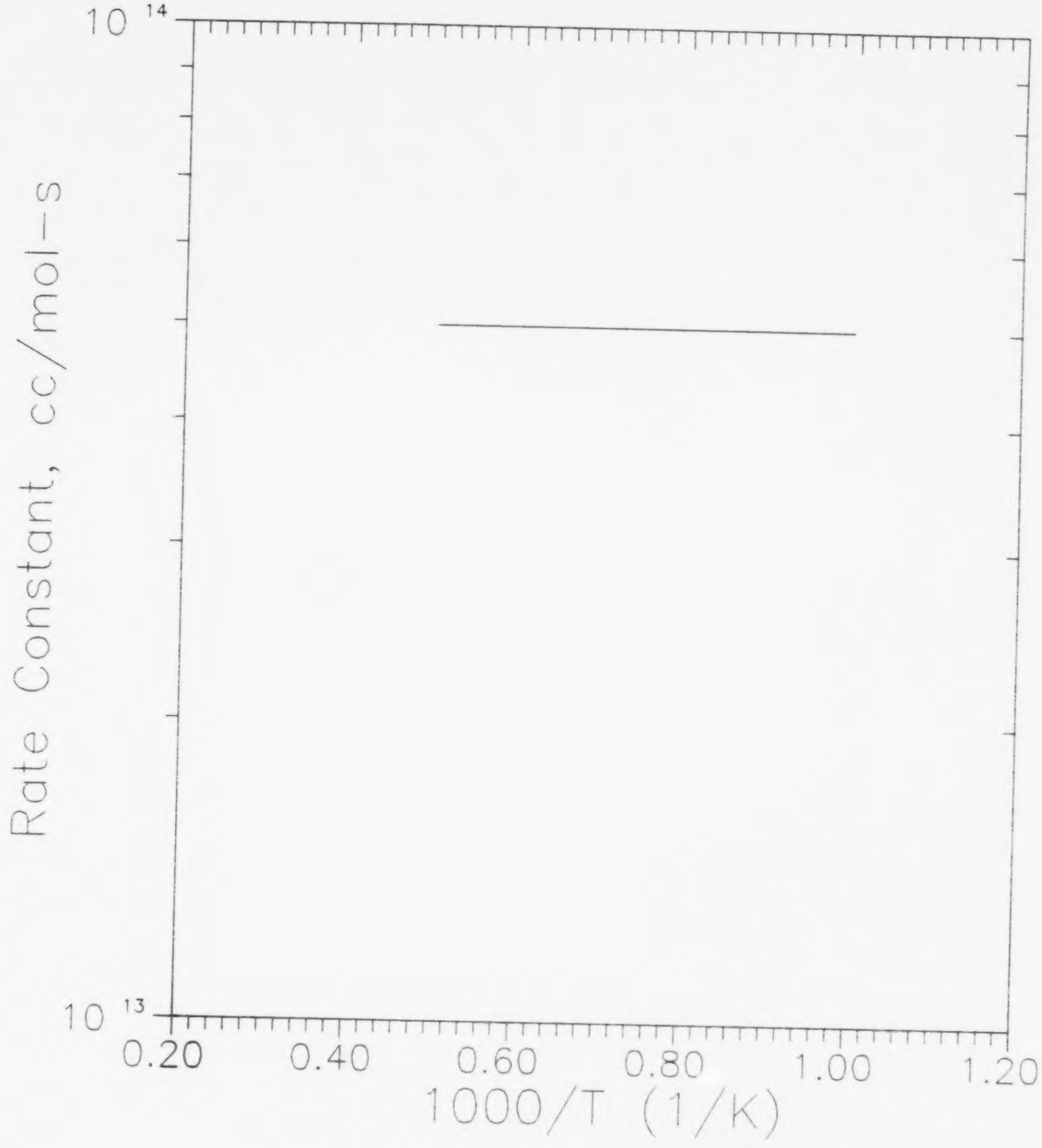
**C2H2 + HO = CH2CO + H**



**C2H2 + HO = CH3 + CO**



**C2H2 + HO = C2H + H2O**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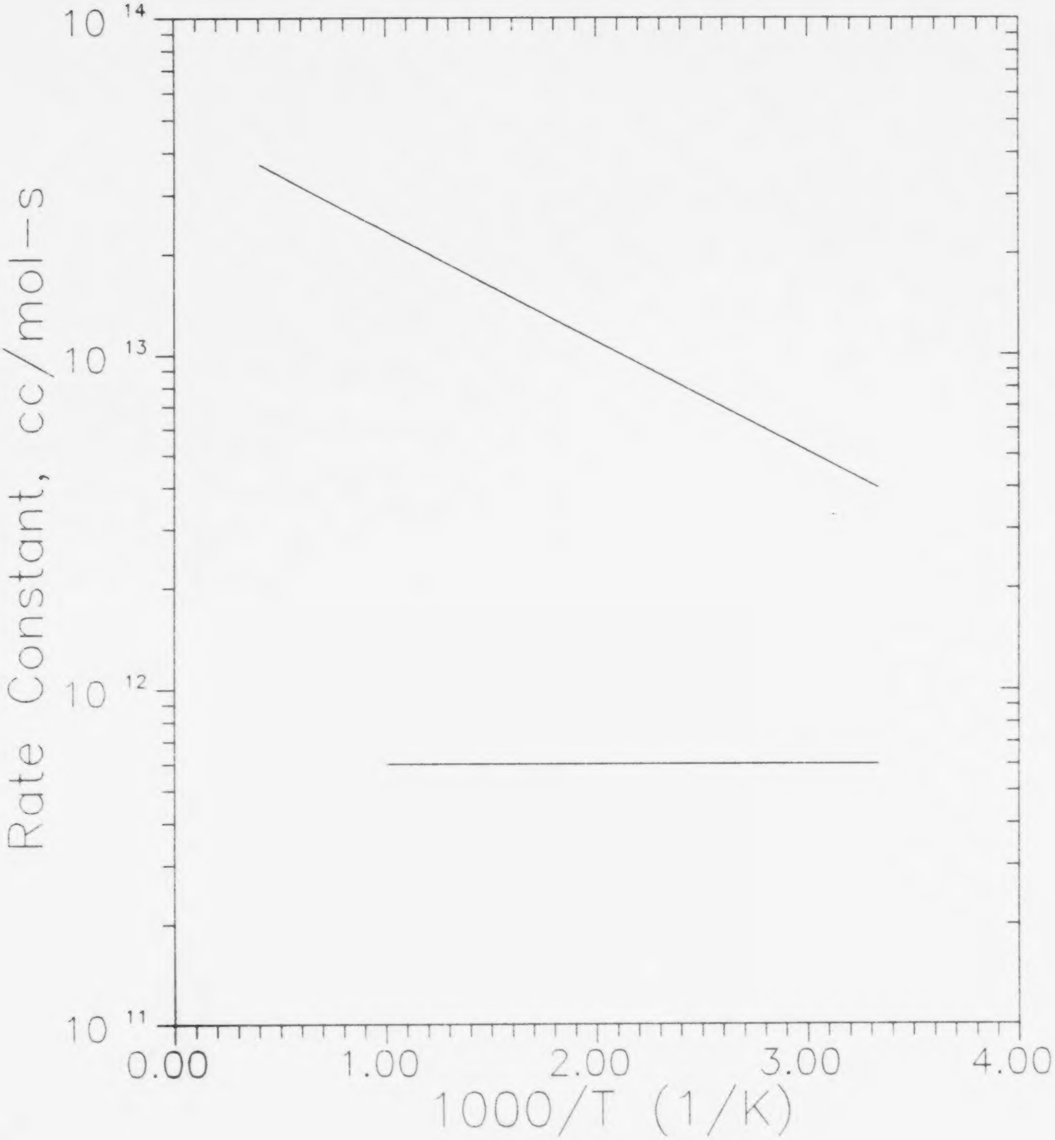
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**C2H + O = CH + CO**



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10 13
10 12
10 11
Rate Constant, cc/mol-s
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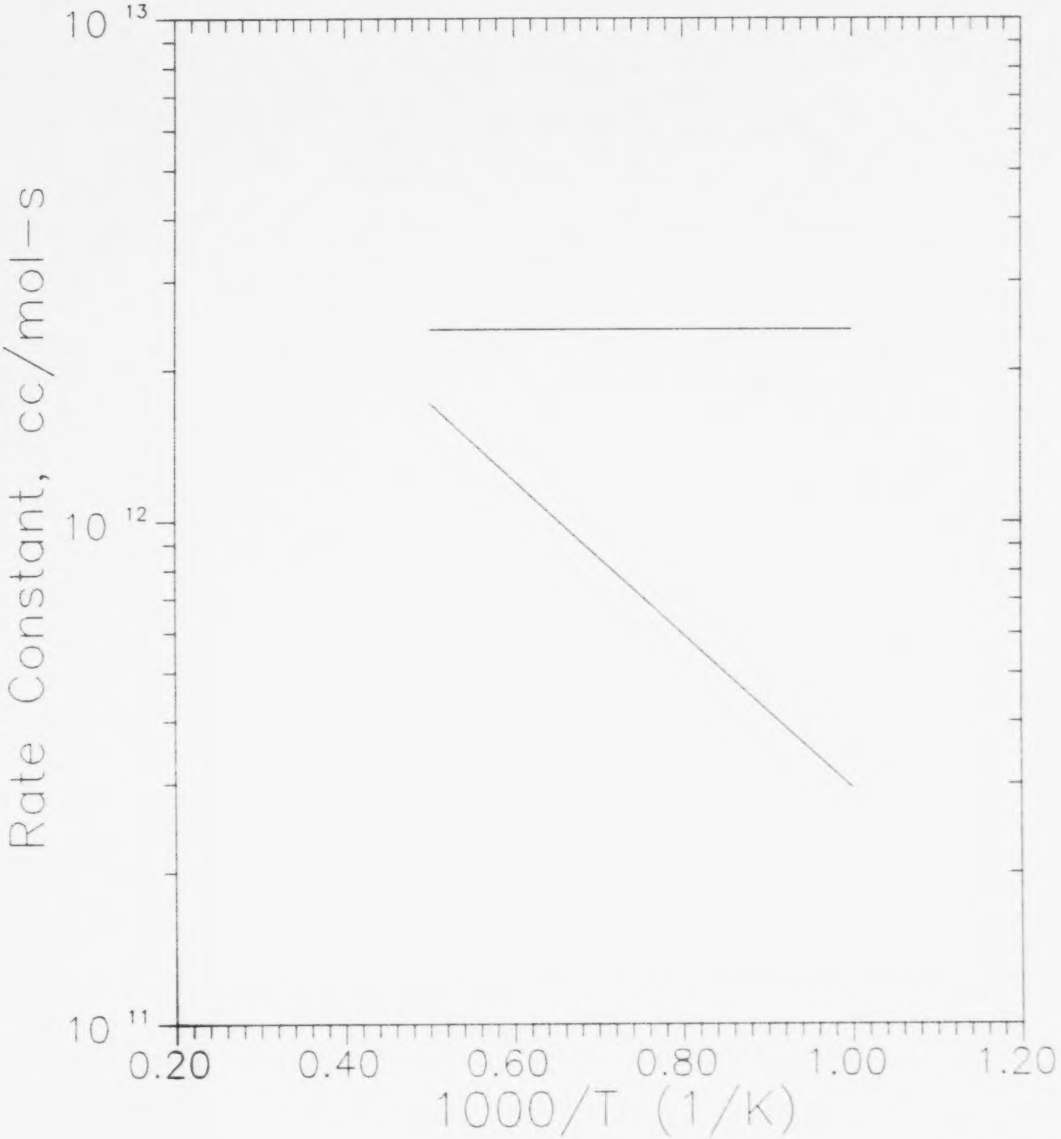
1.00
2.00
3.00
4.00
1000/T (1/K)

**C2H + O2 = CHCO + O**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10 12
10 11
Rate Constant, cc/mol-s
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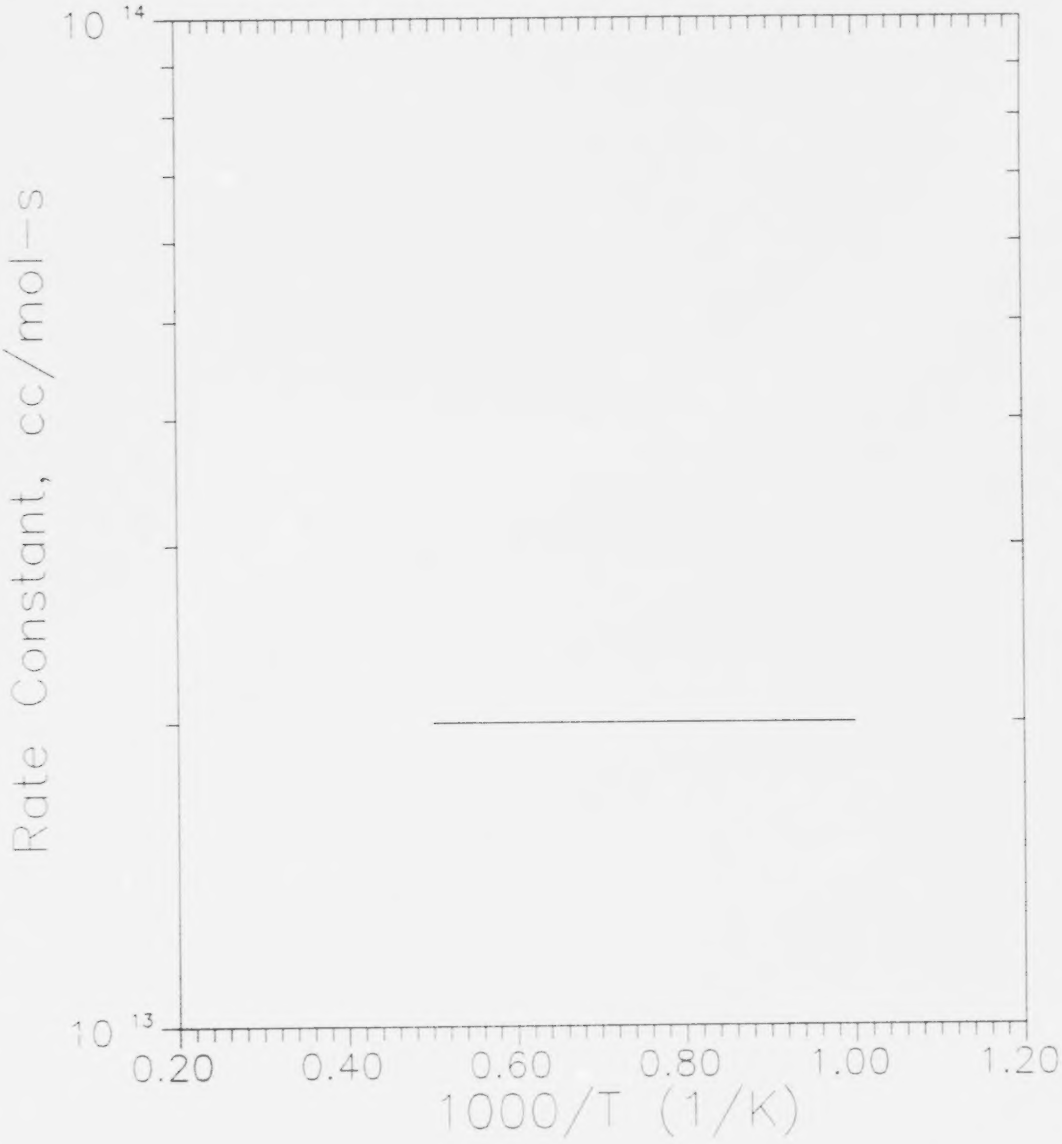
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**C2H + O2 = CHO + CO**



$10^{14}$
$10^{13}$
Rate Constant, cc/mol-s
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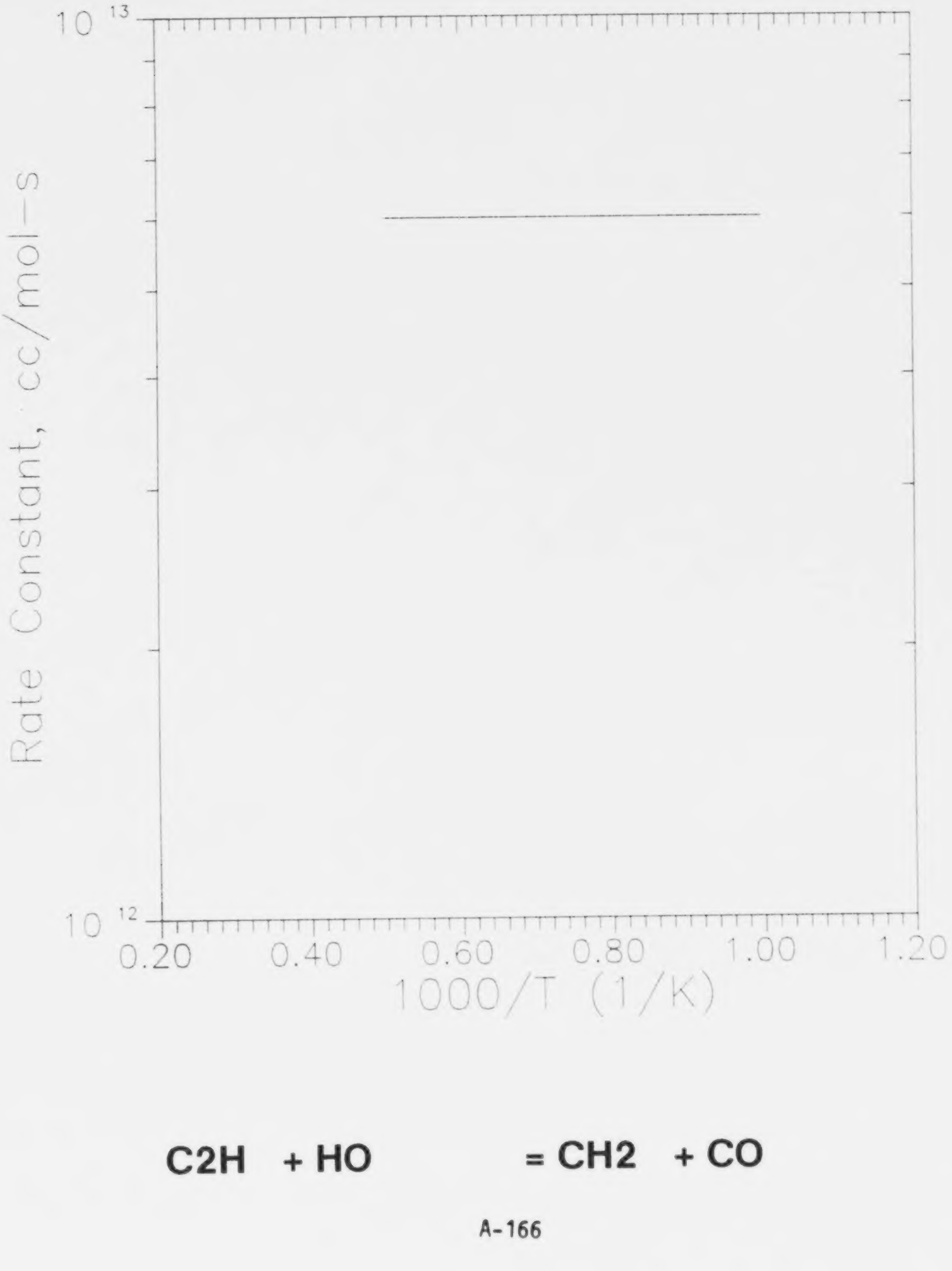
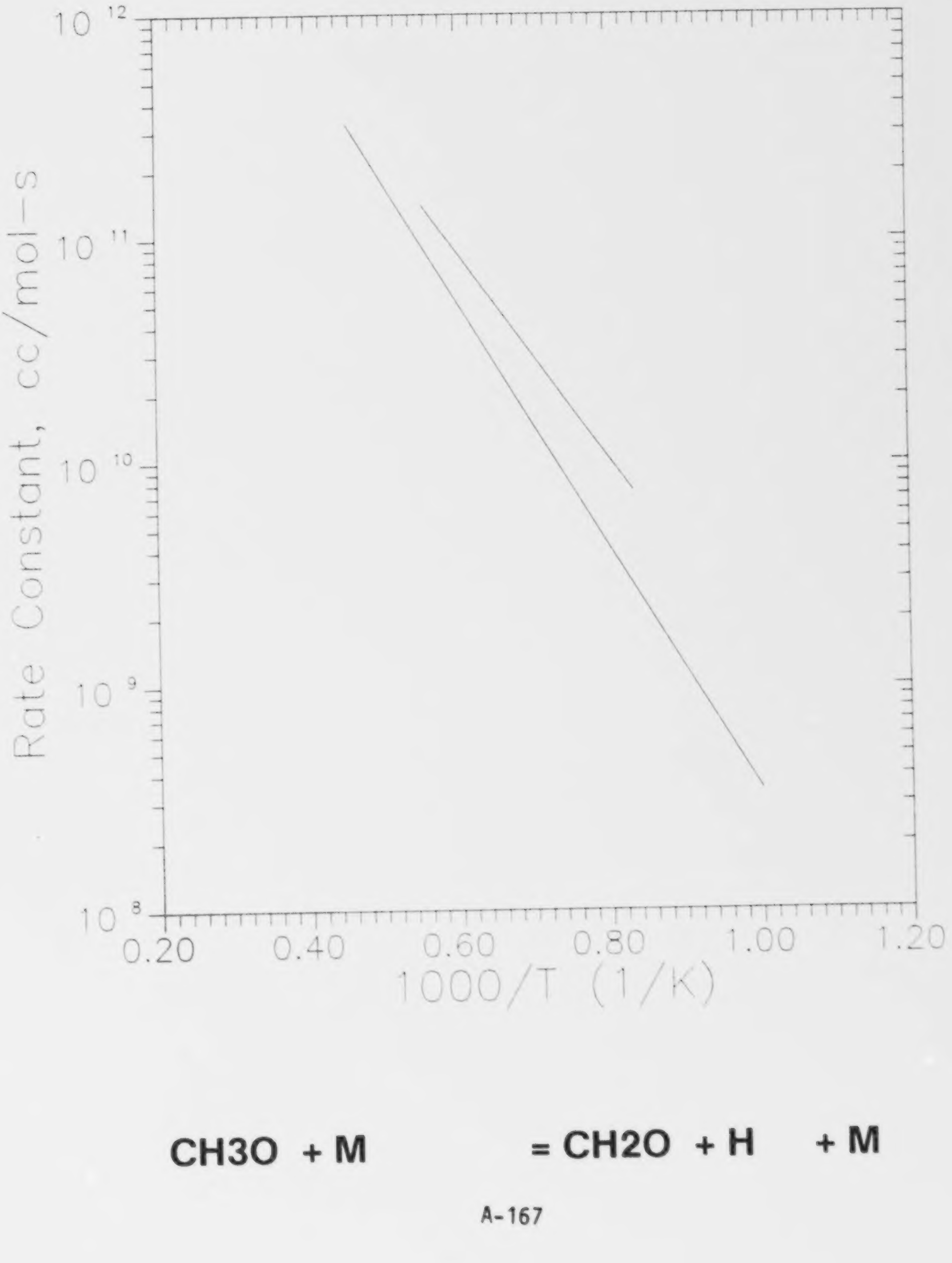
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

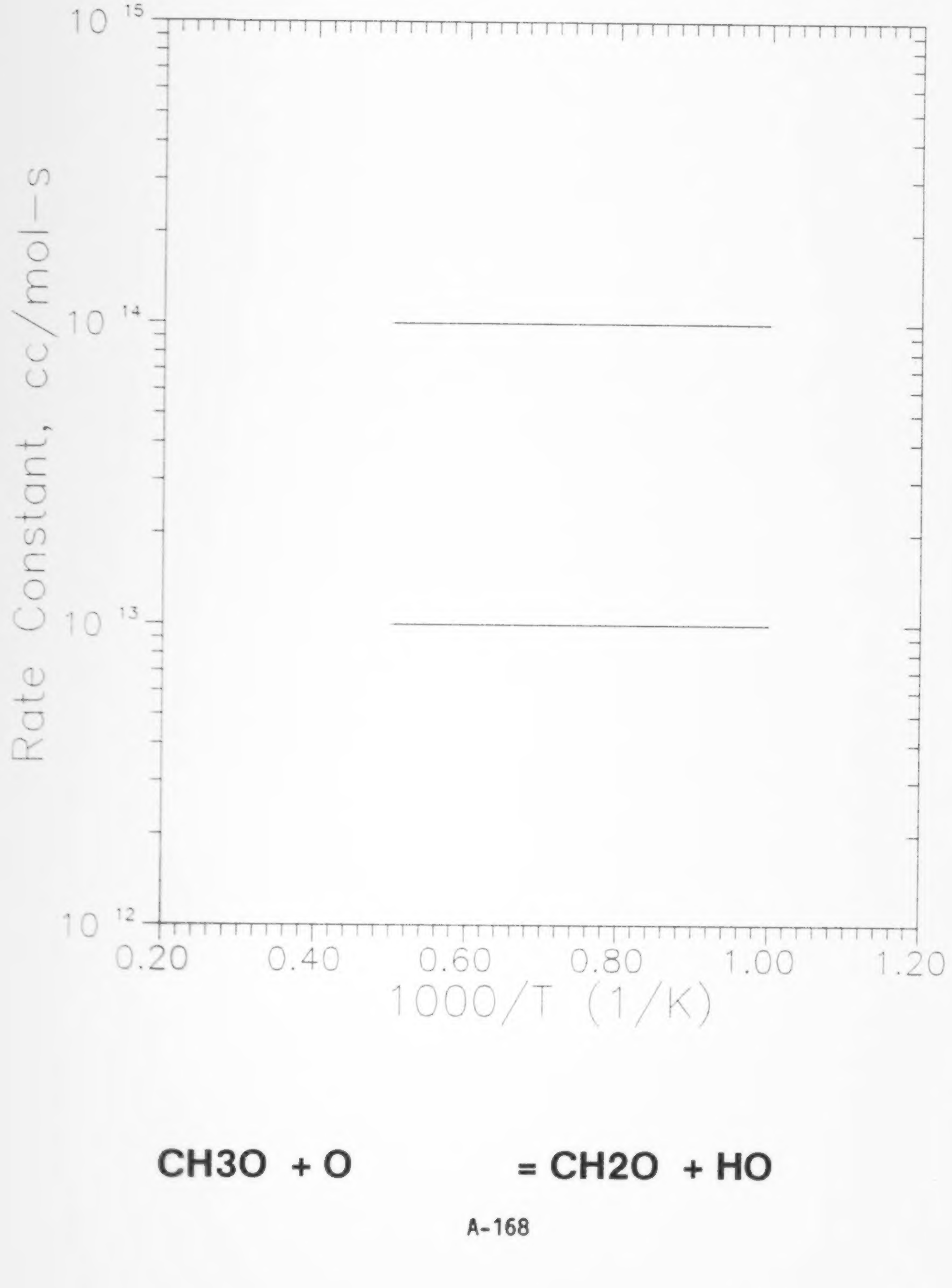
**C2H + HO = CHCO + H**


10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

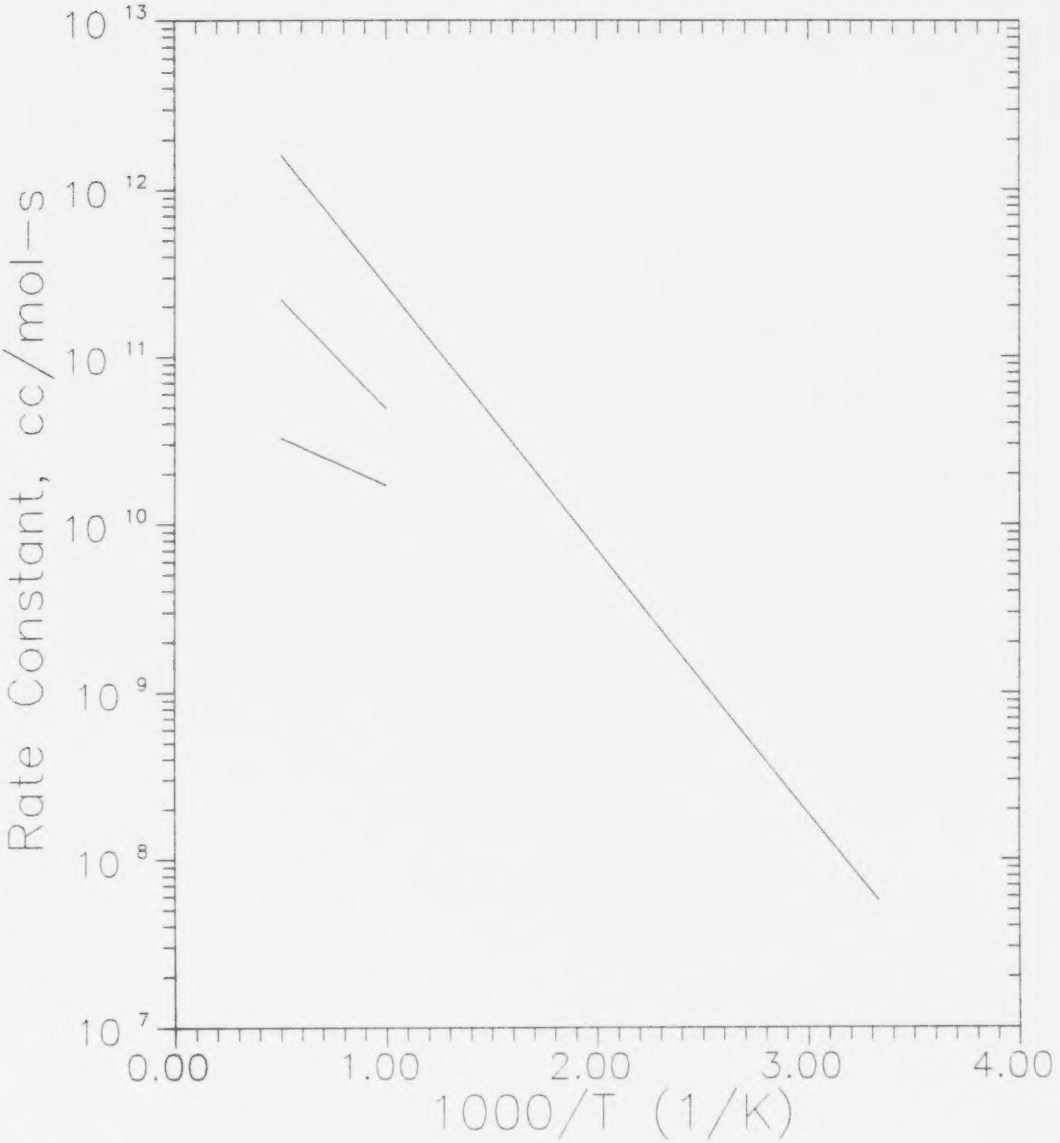
**C2H + HO = CH2 + CO**



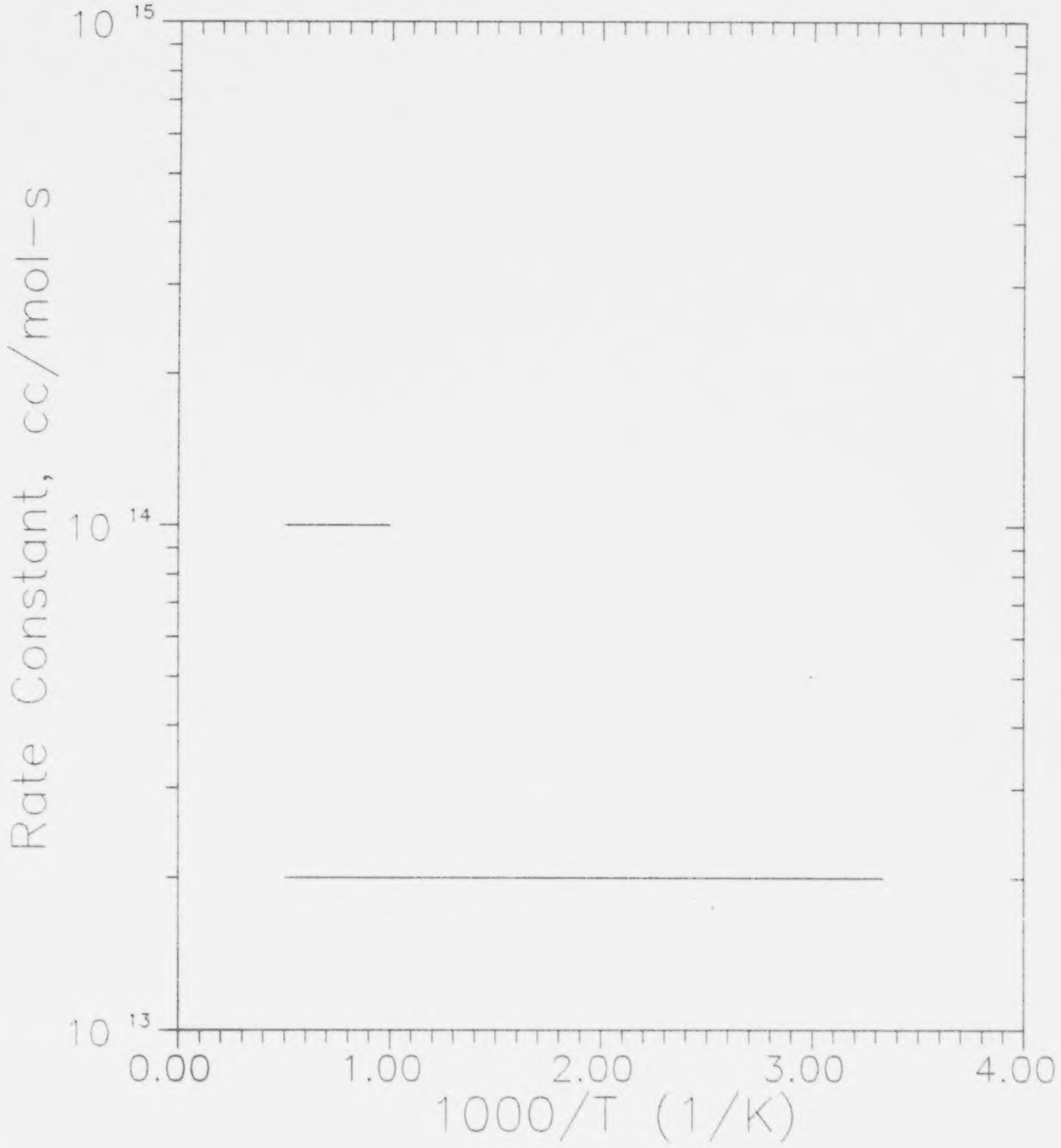
**CH3O + M = CH2O + H + M**



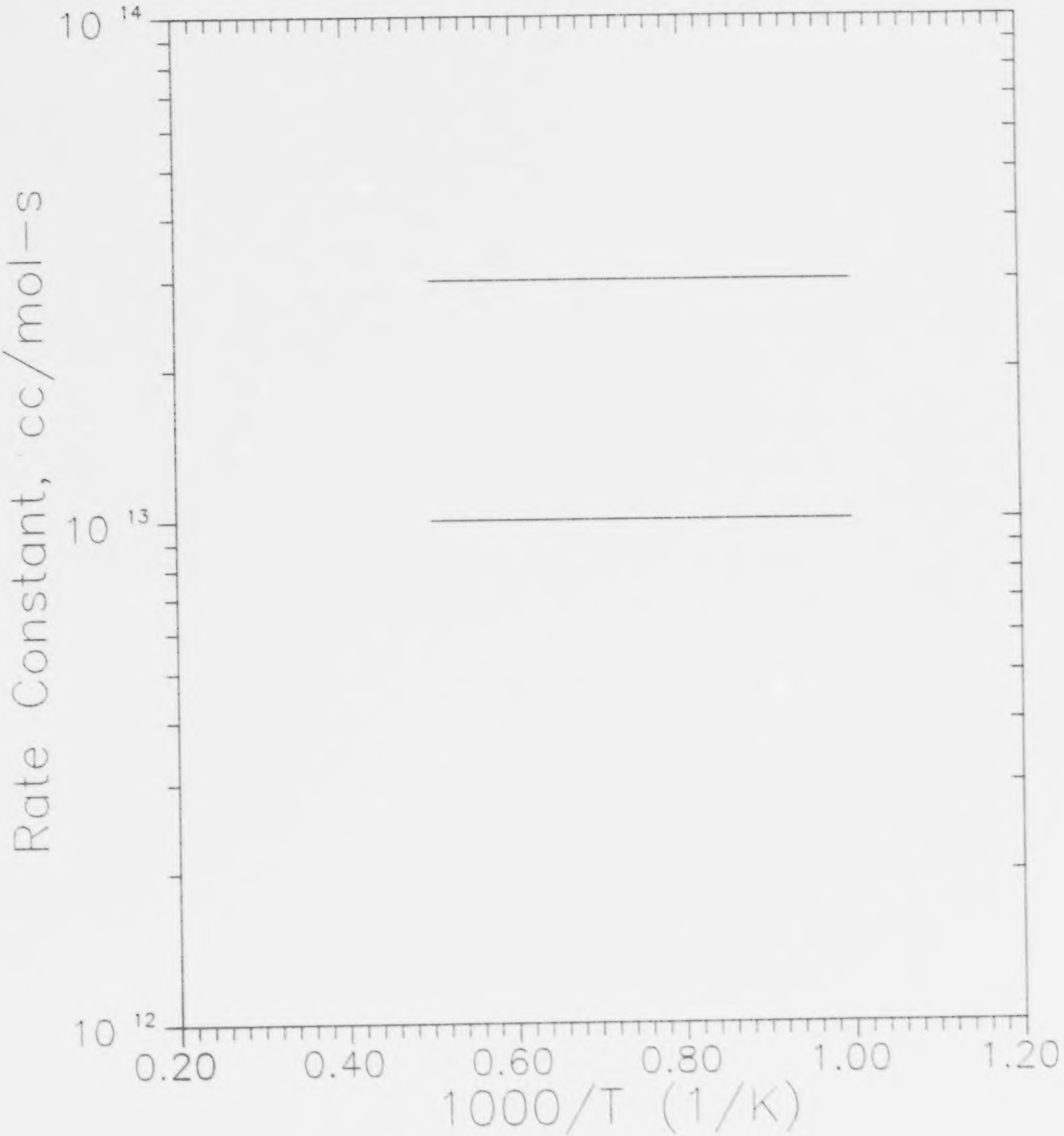
**CH3O + O = CH2O + HO**



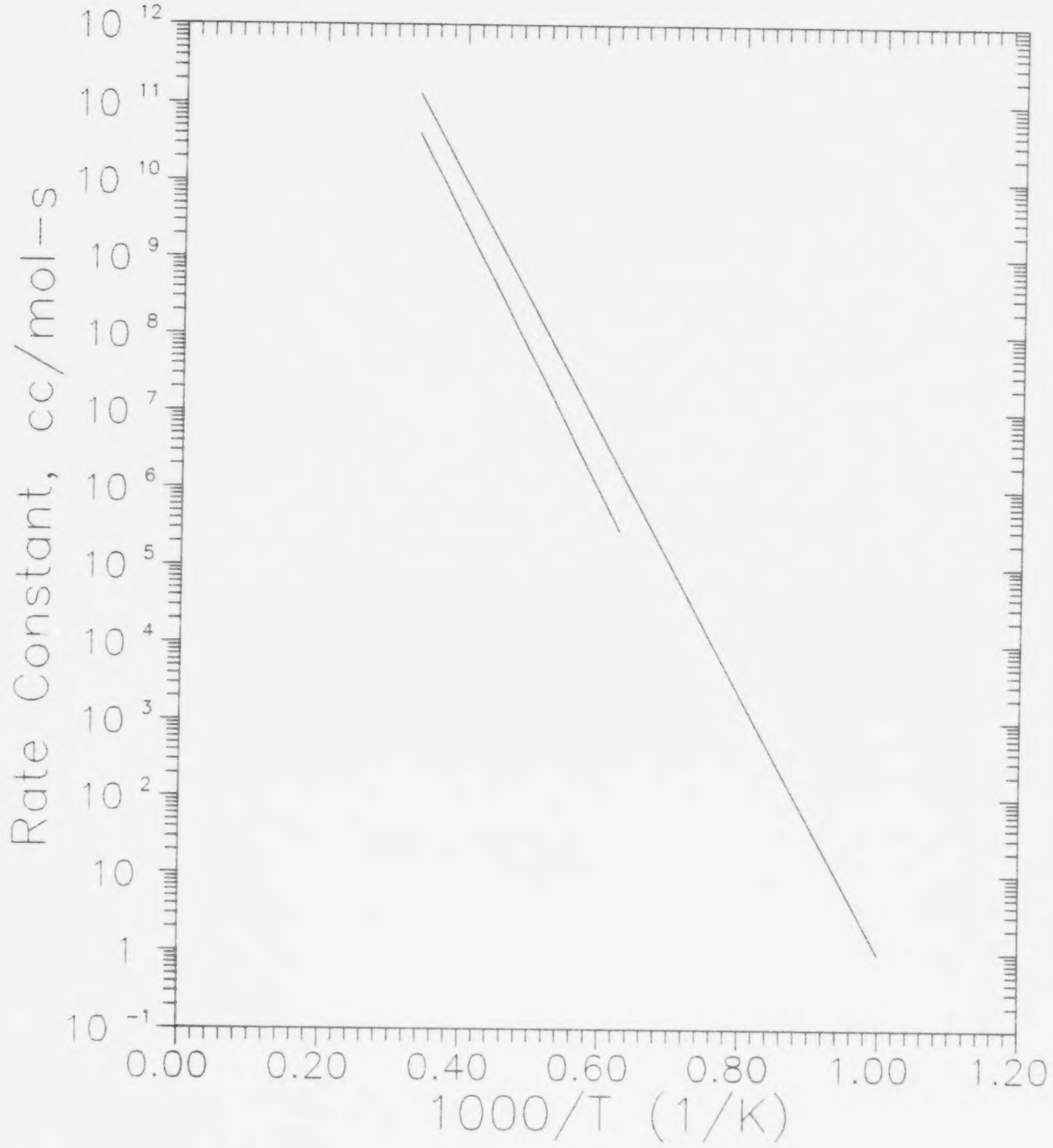
**CH3O + O2 = CH2O + HO2**



**CH3O + H = CH2O + H2**



**$CH_3O$ + $HO$ = $CH_2O$ + $H_2O$**



Rate Constant, cc/mol-s
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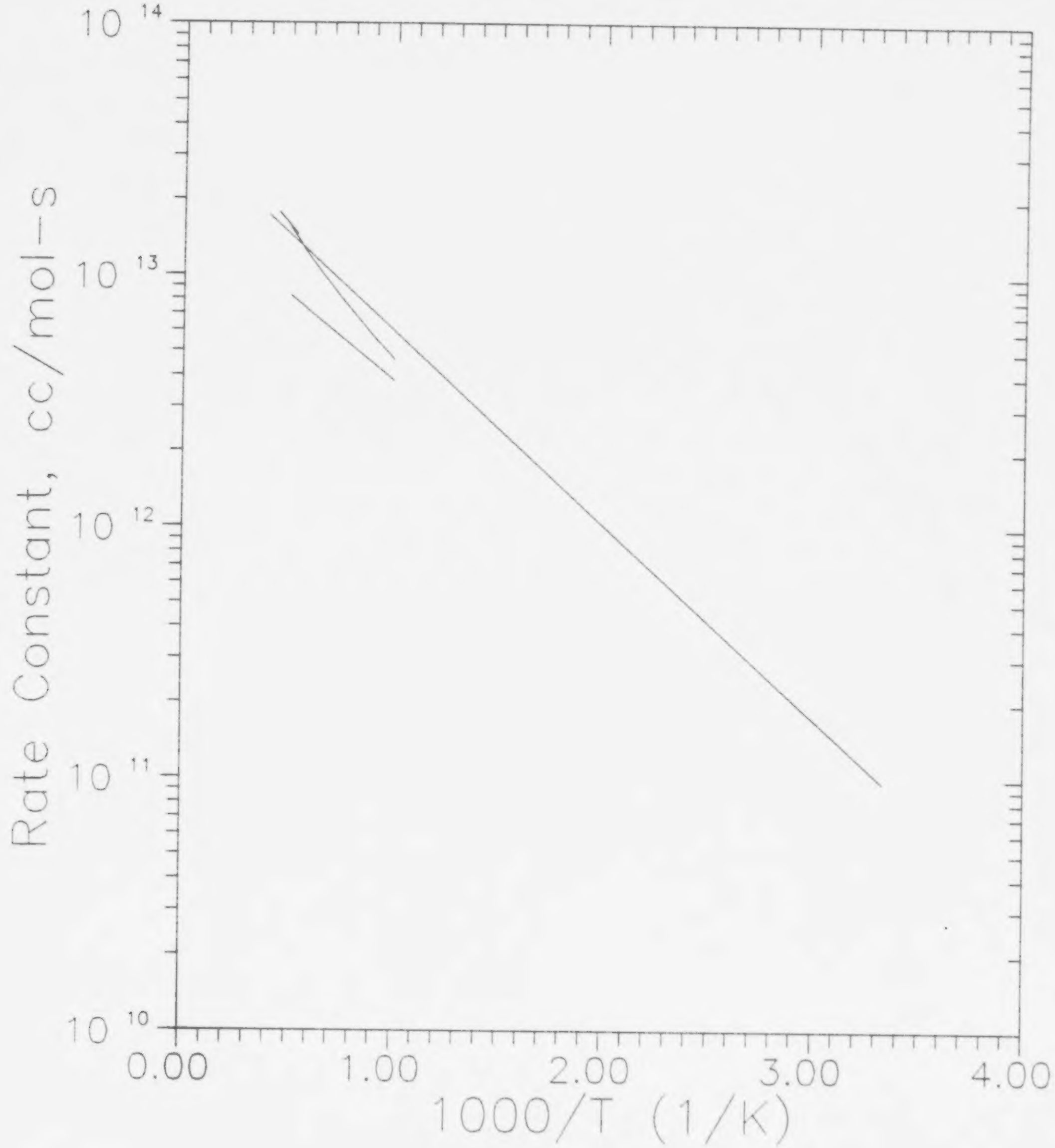
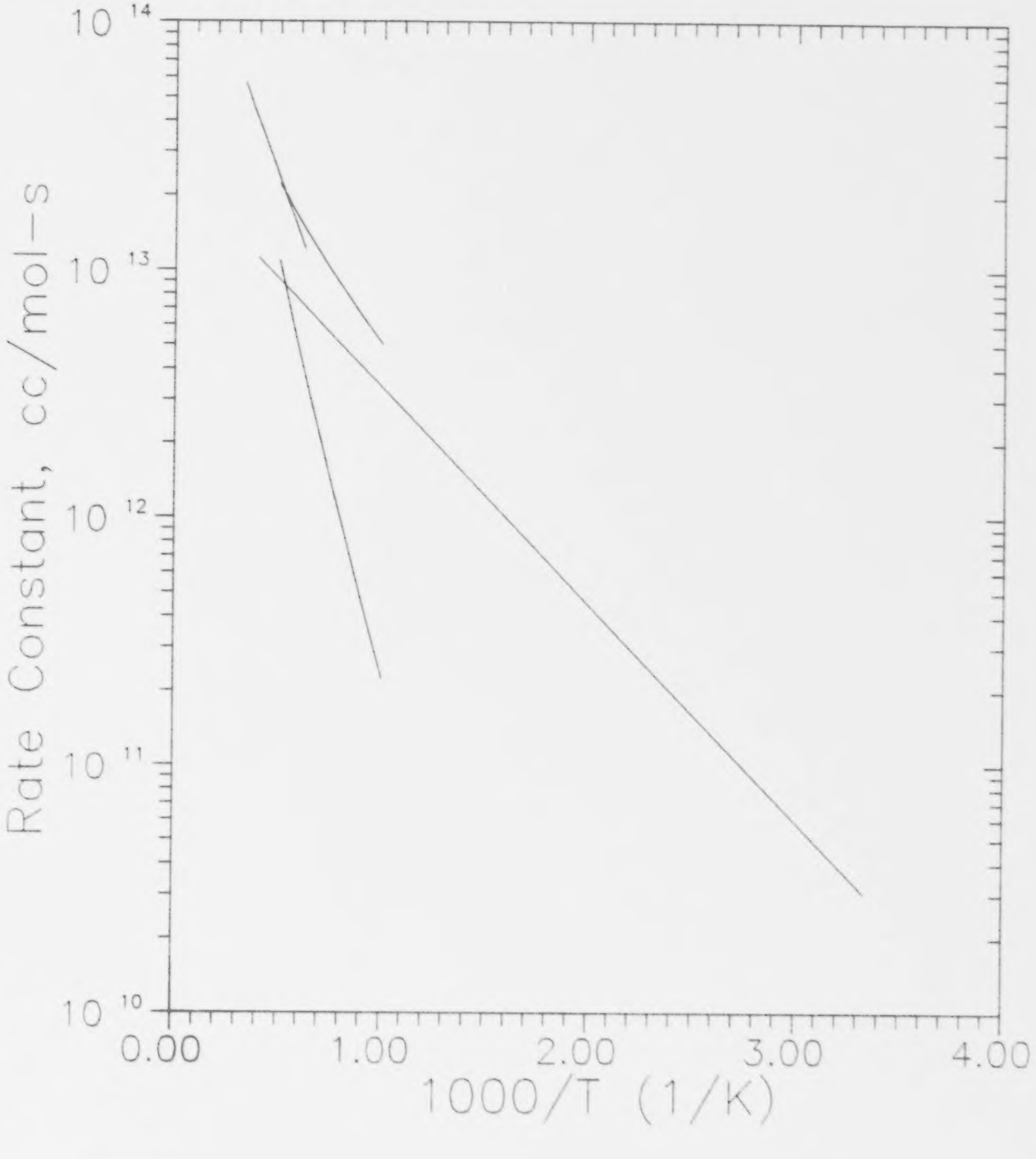
$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
$10^{5}$
$10^{4}$
$10^{3}$
$10^{2}$
10
1
$10^{-1}$
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2O + M = CHO + H + M**

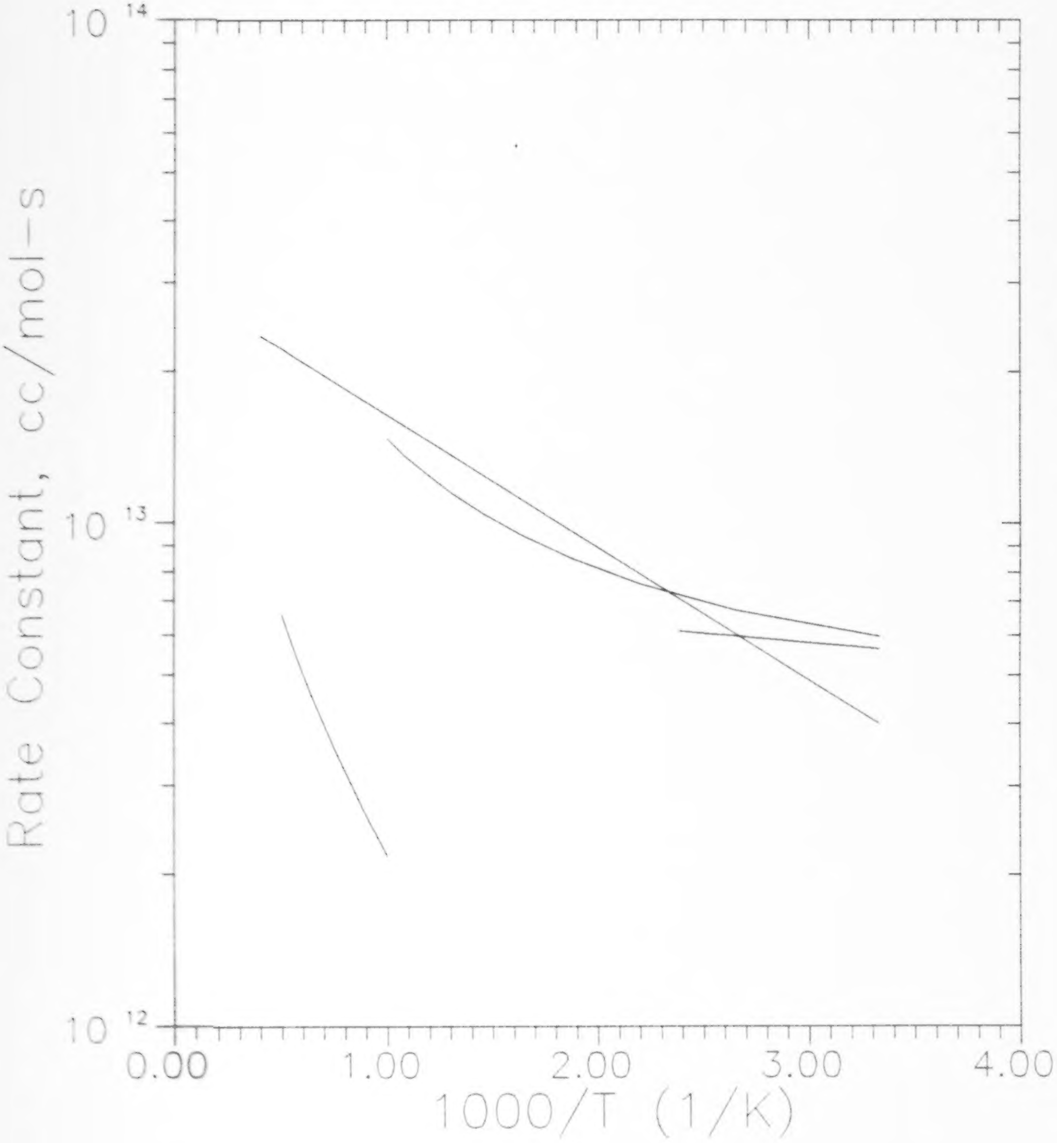

10 14
10 13
10 12
10 11
10 10
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**CH2O + O = CHO + HO**

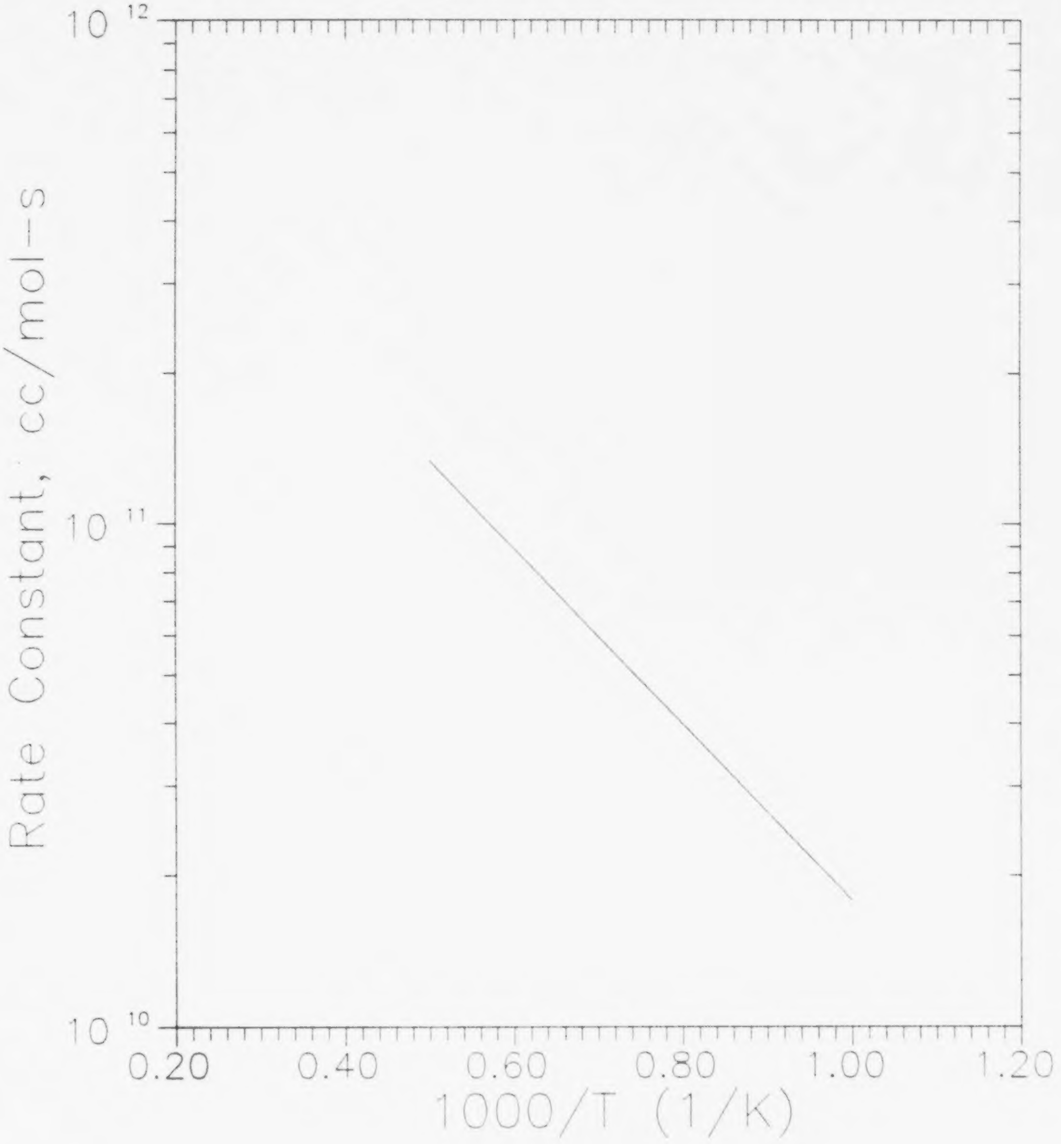


Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
$10^{10}$
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

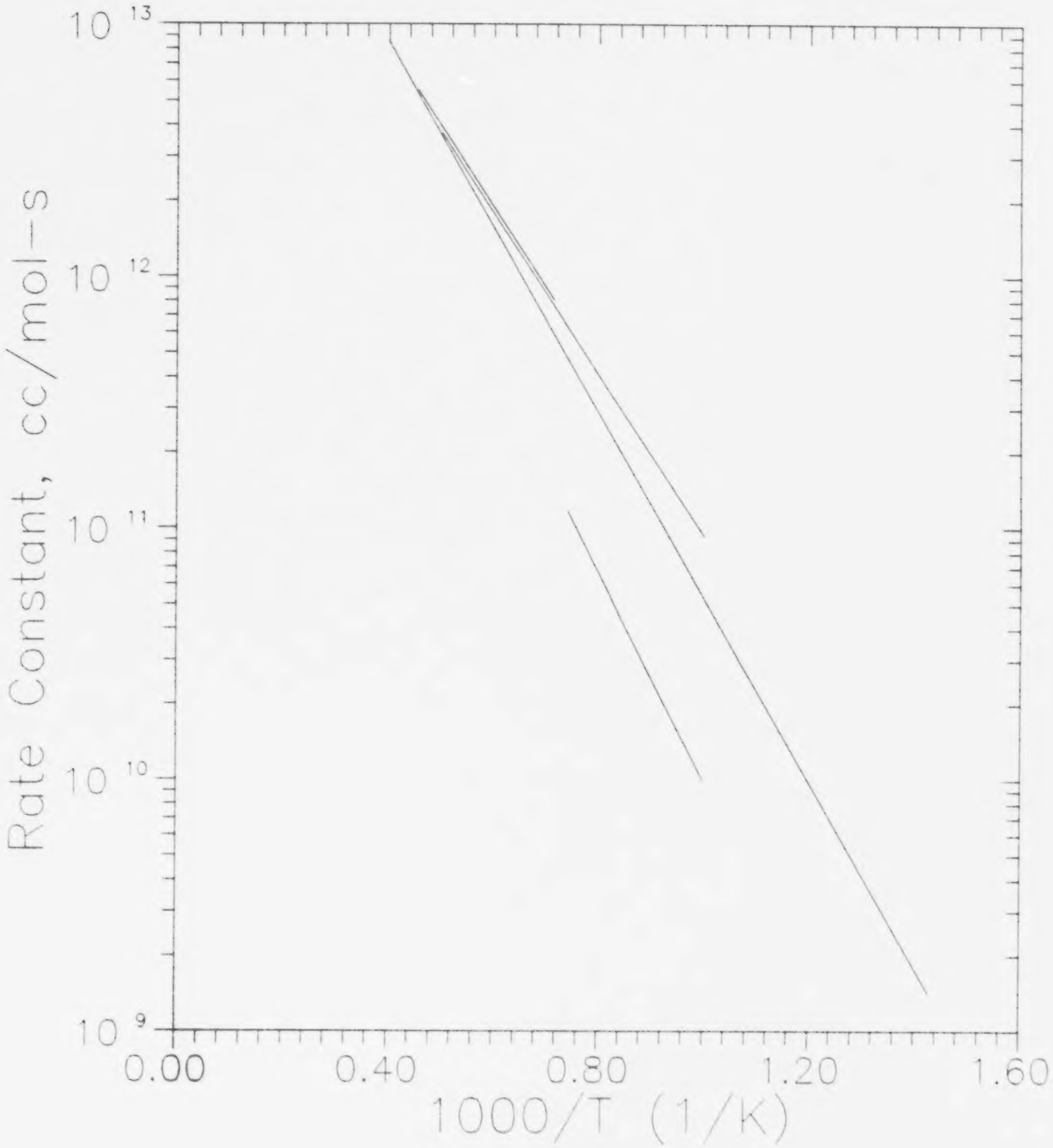
**CH2O + H = CHO + H2**



**CH2O + HO = CHO + H2O**



**CH2O + HO2 = CHO + H2O2**



$10^{13}$
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
Rate Constant, cc/mol-s
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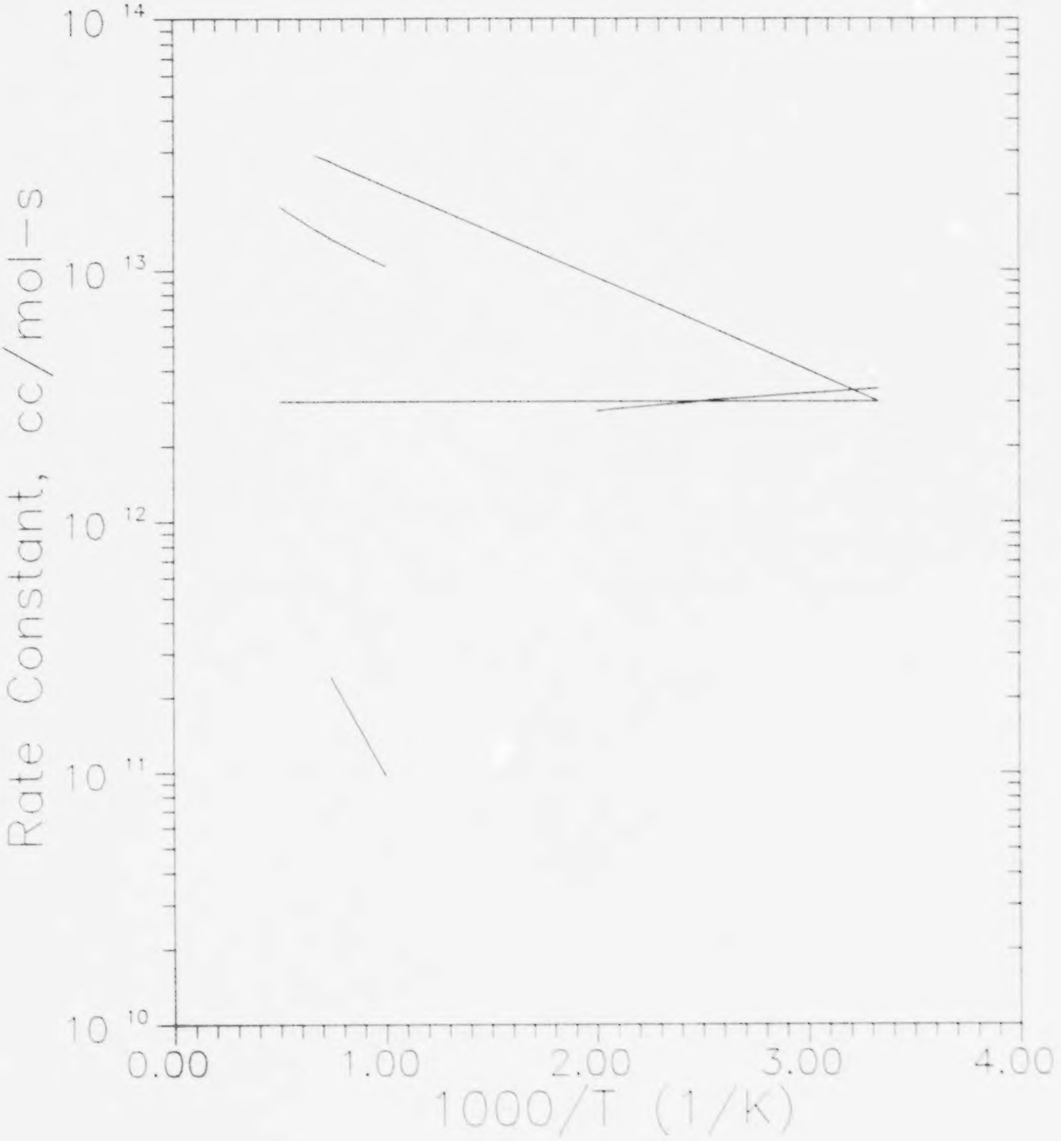
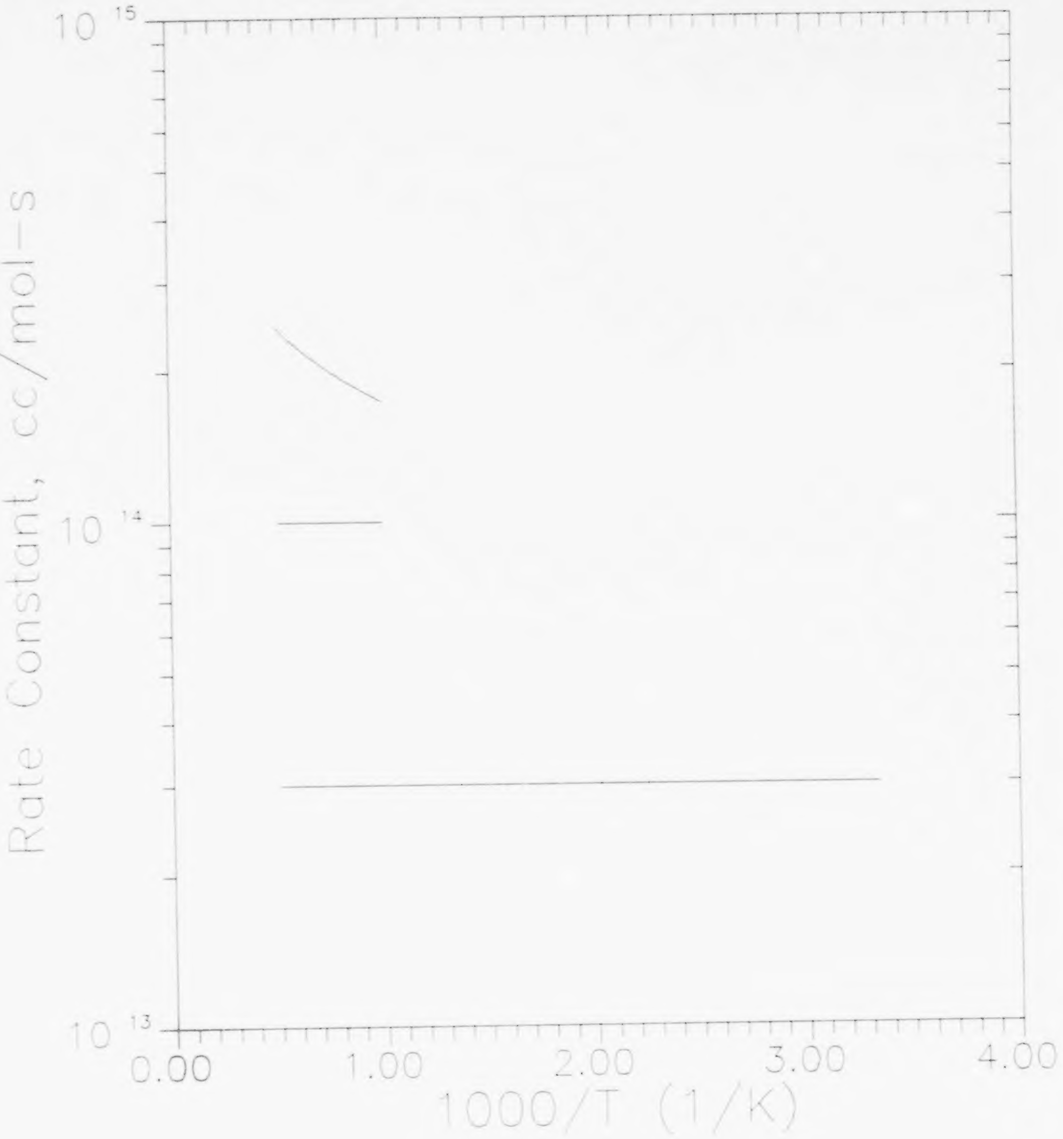
0.40
0.80
1.20
1.60
1000/T (1/K)

**CHO + M = CO + H + M**



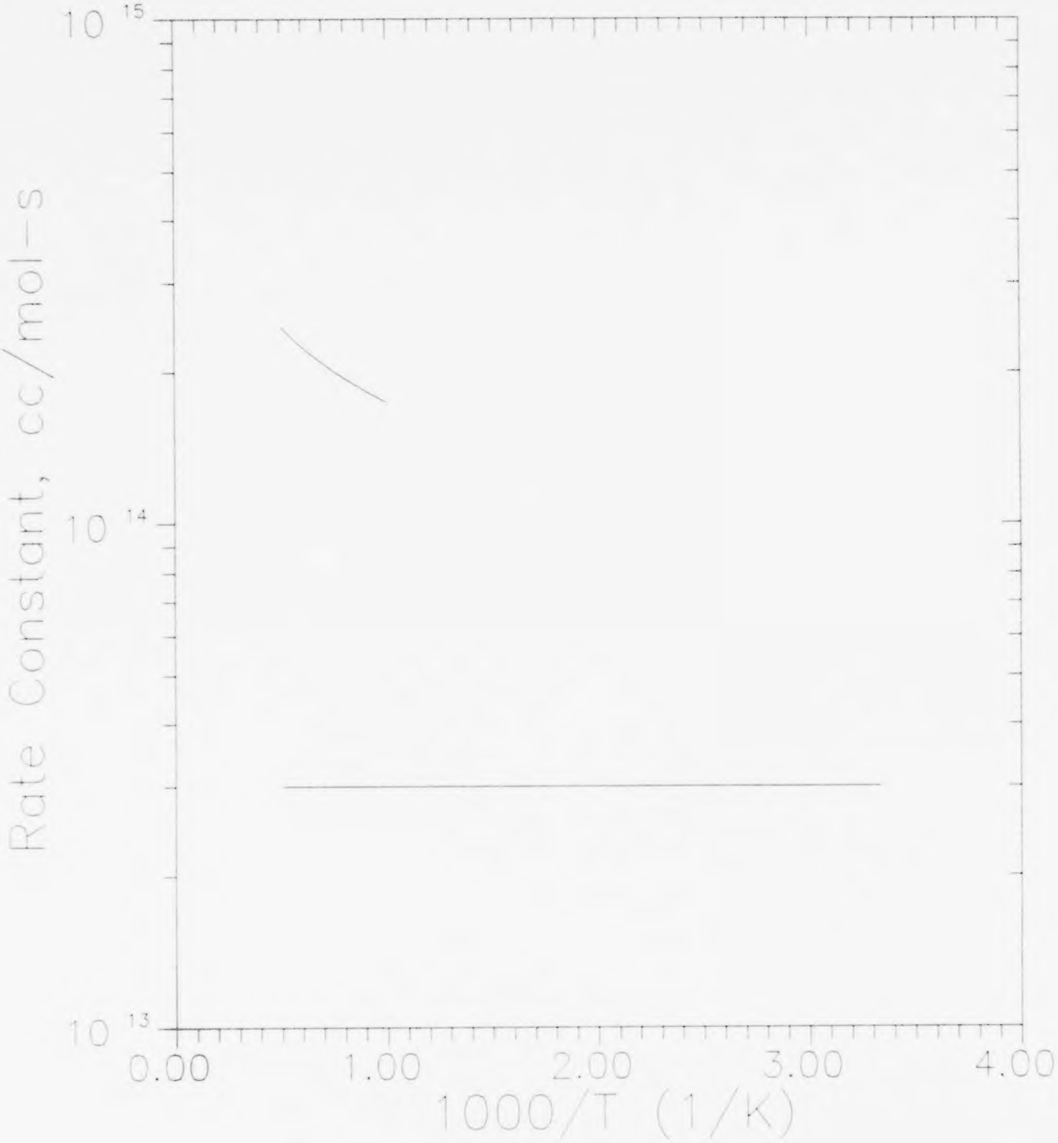
Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
$10^{10}$
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**CHO + O2 = CO + HO2**

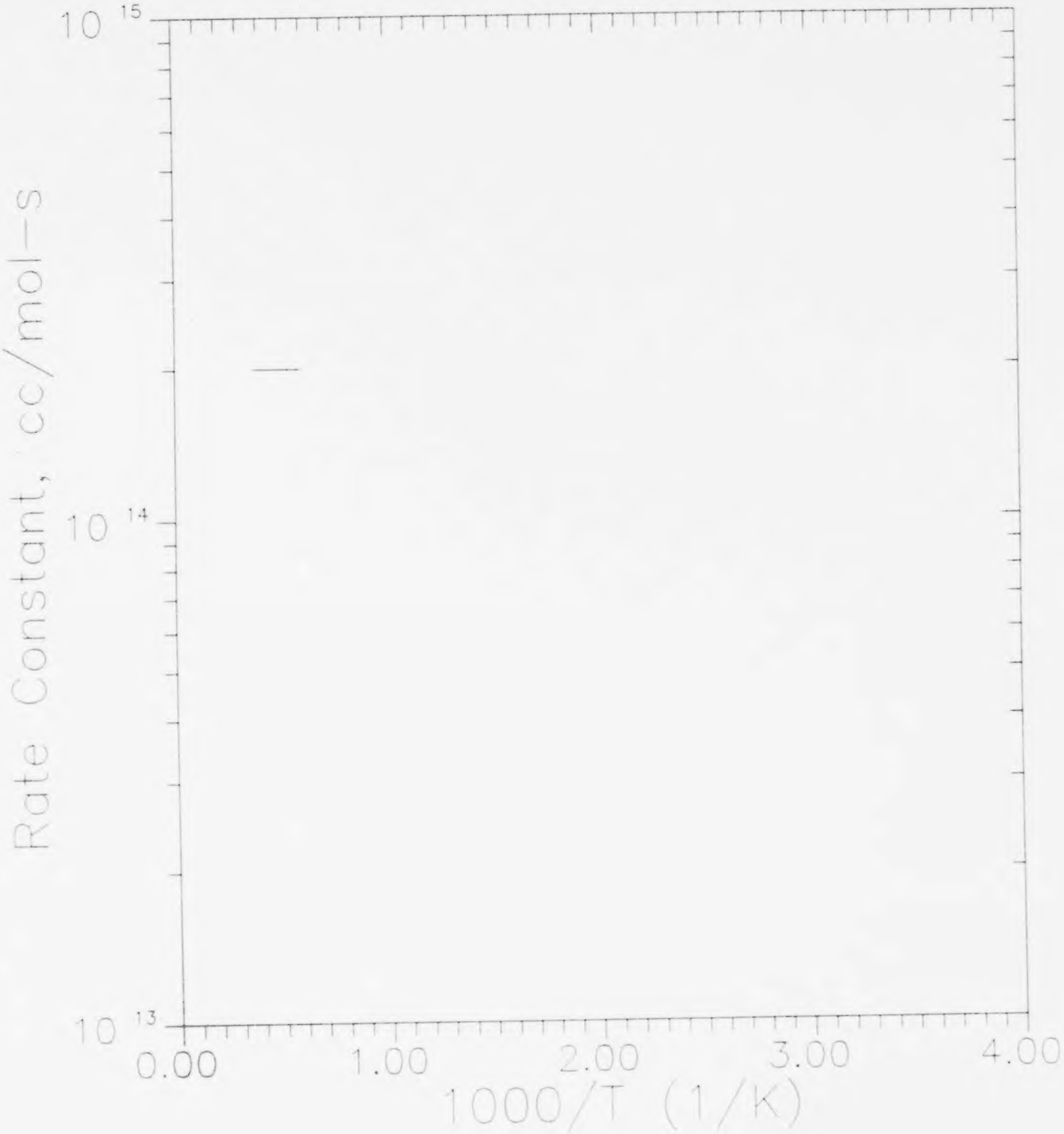


10^15
10^14
10^13
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

CHO + O = CO + HO


10^15
10^14
10^13
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**CHO + O = CO2 + H**


Rate Constant, cc/mol-s
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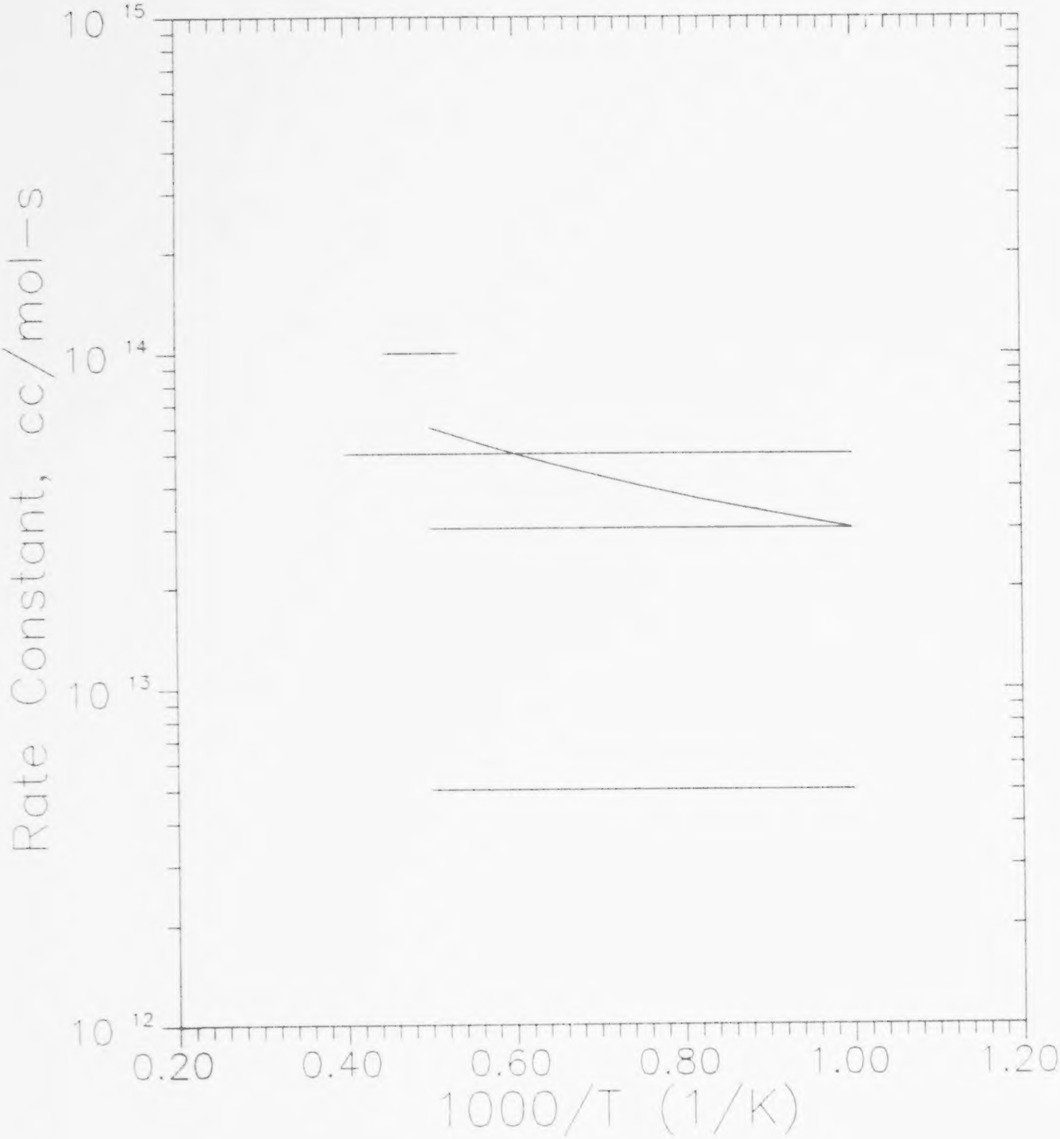
10 14
10 13
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**CHO + H = CO + H2**


10 15
10 14
10 13
10 12
Rate Constant, cc/mol-s
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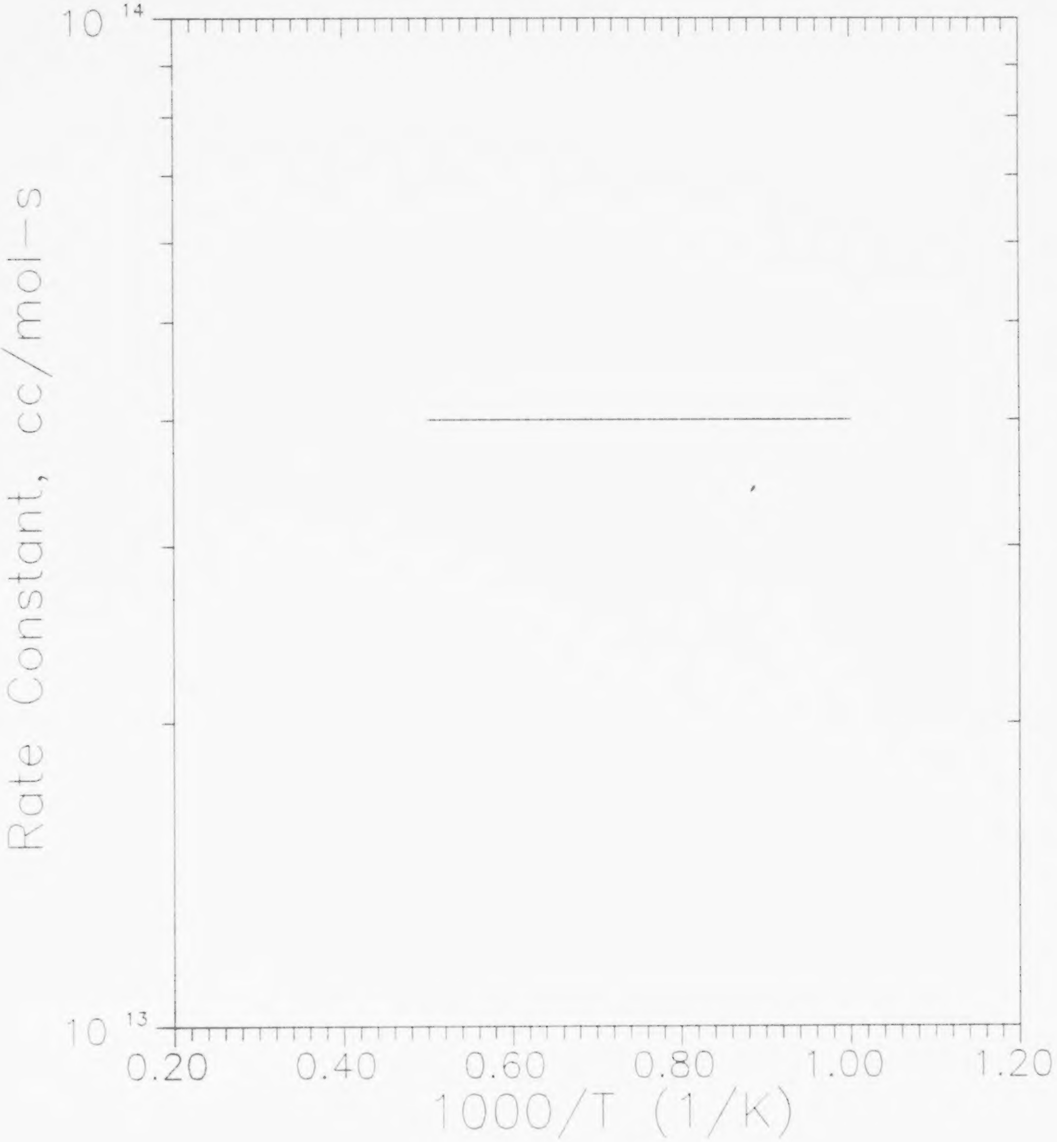
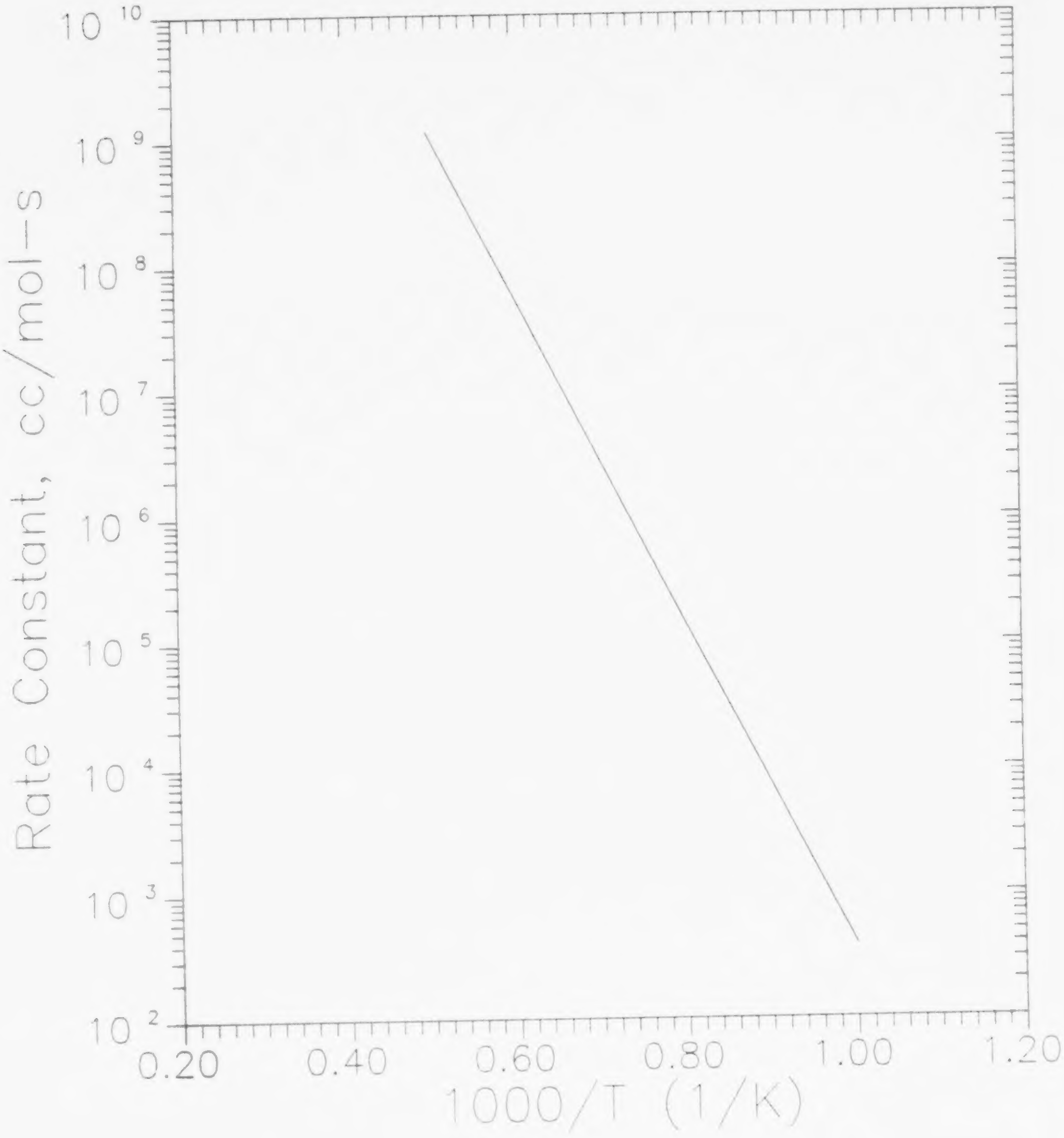
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

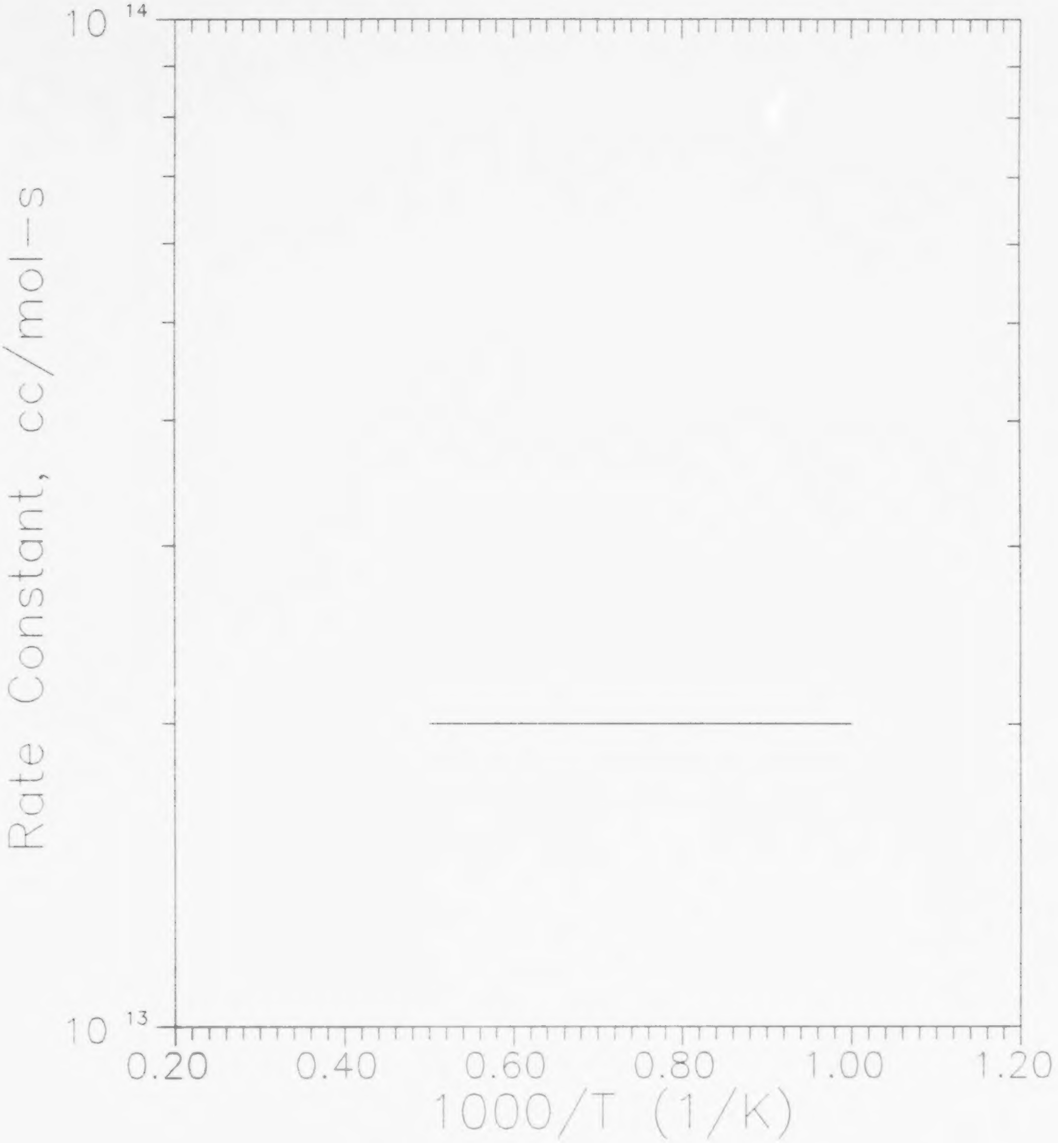
**CHO + HO = CO + H2O**



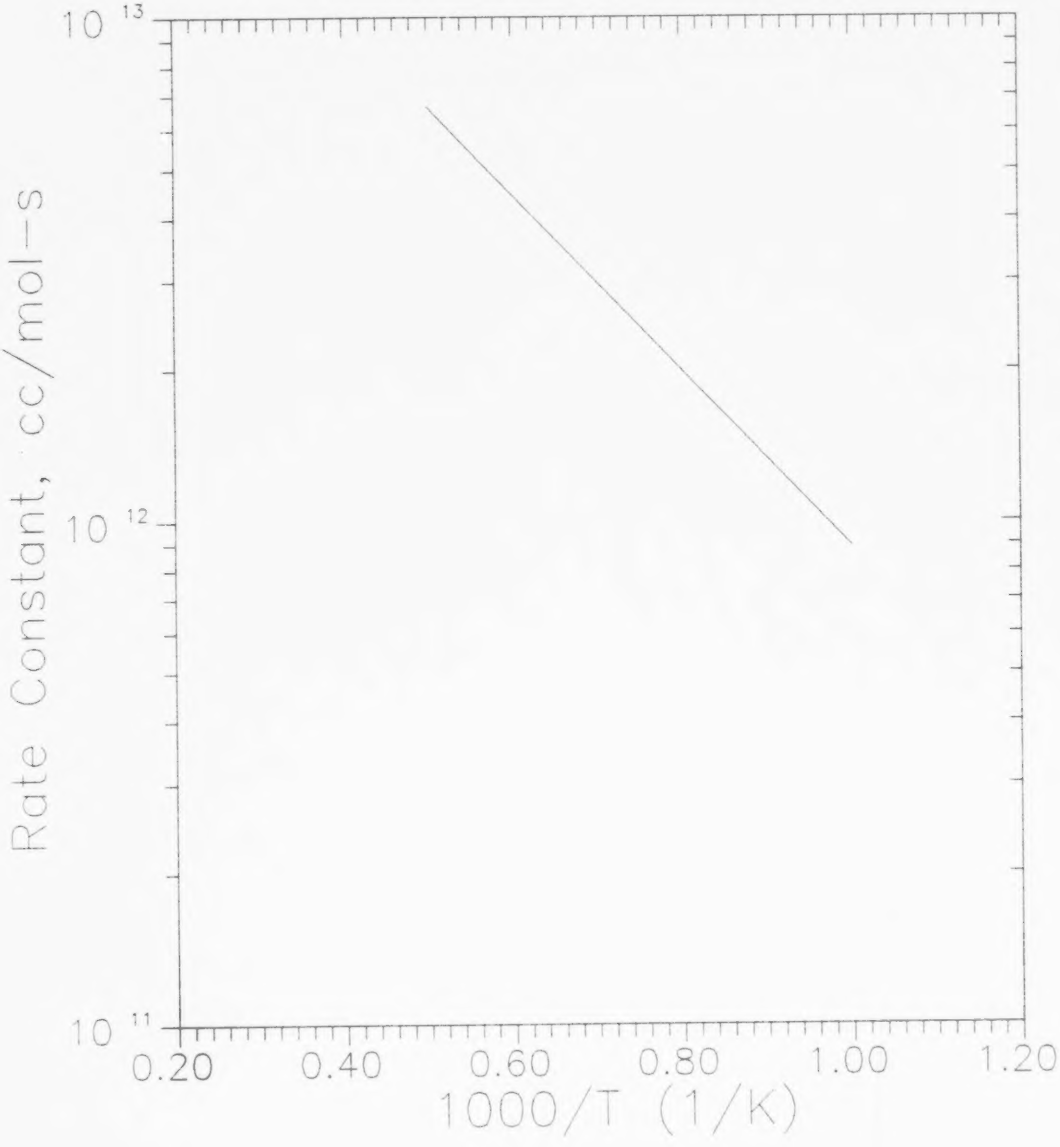
**CHO + CHO = CO + CH2O**



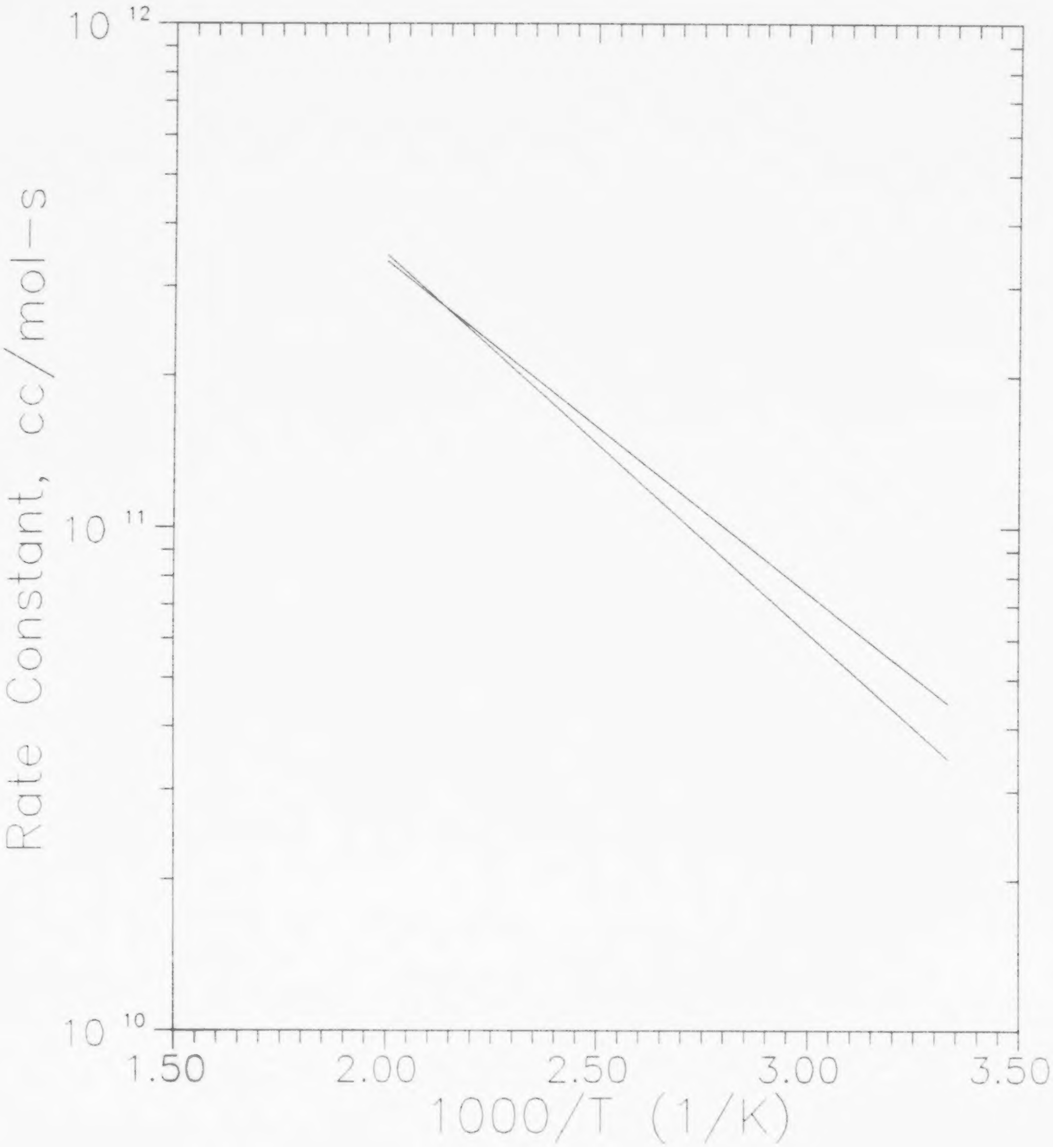
**CH2CO + M = CH2 + CO + M**



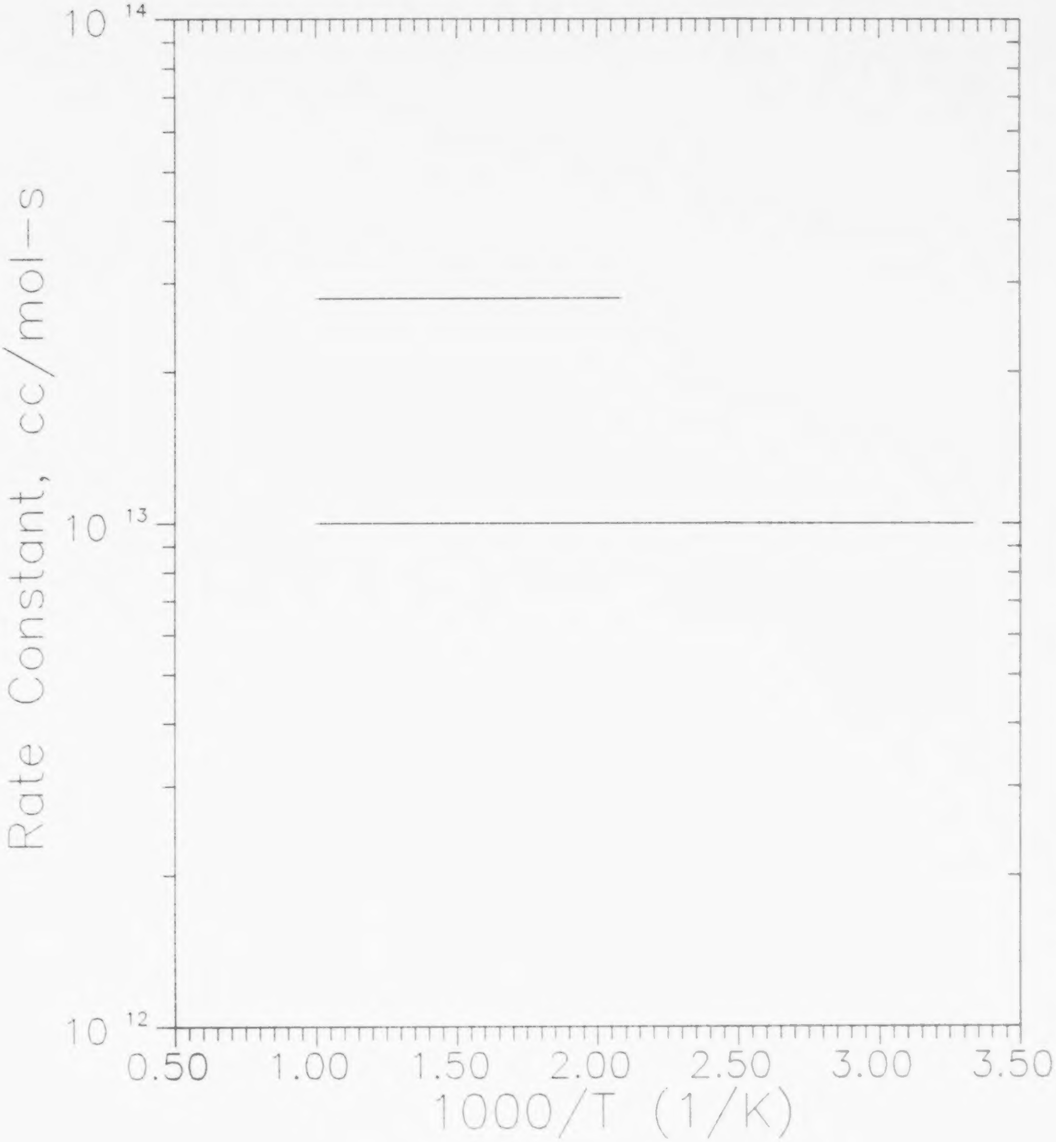
**CH2CO + O = CH2O + CO**



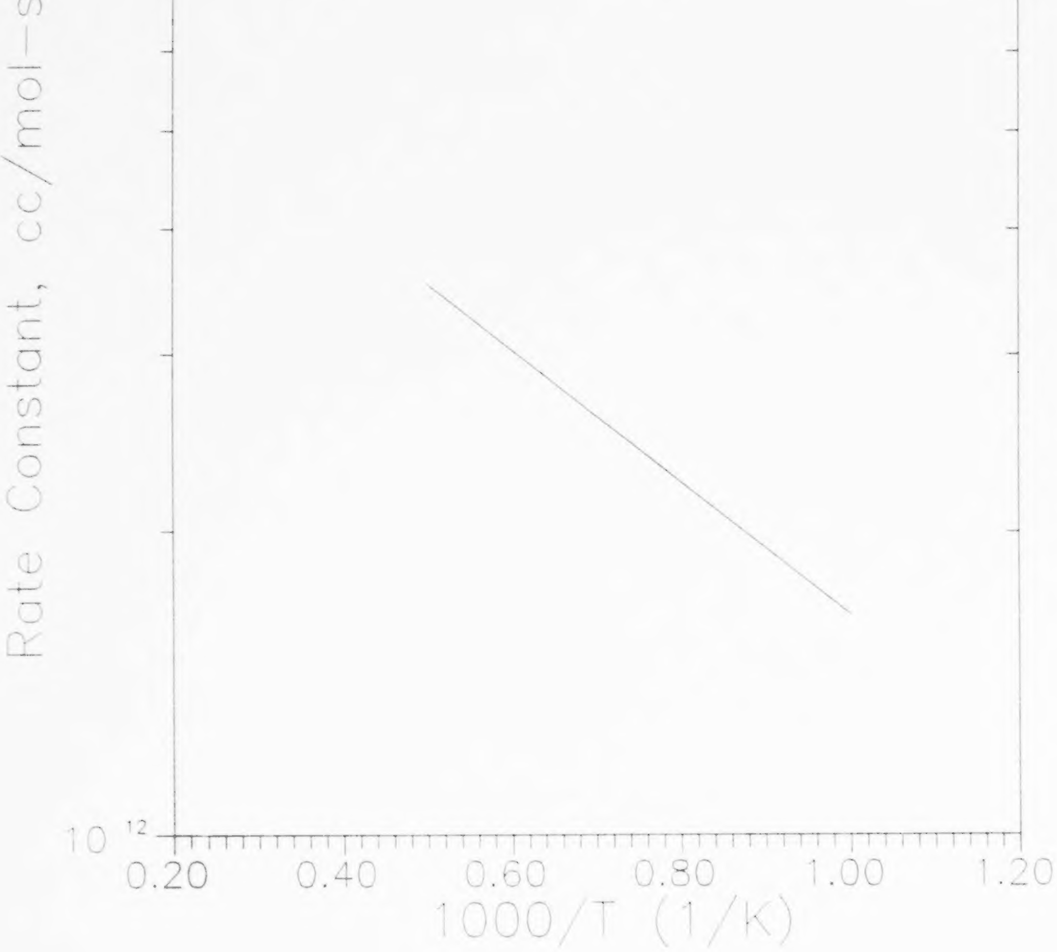
**CH2CO + O = CHCO + HO**



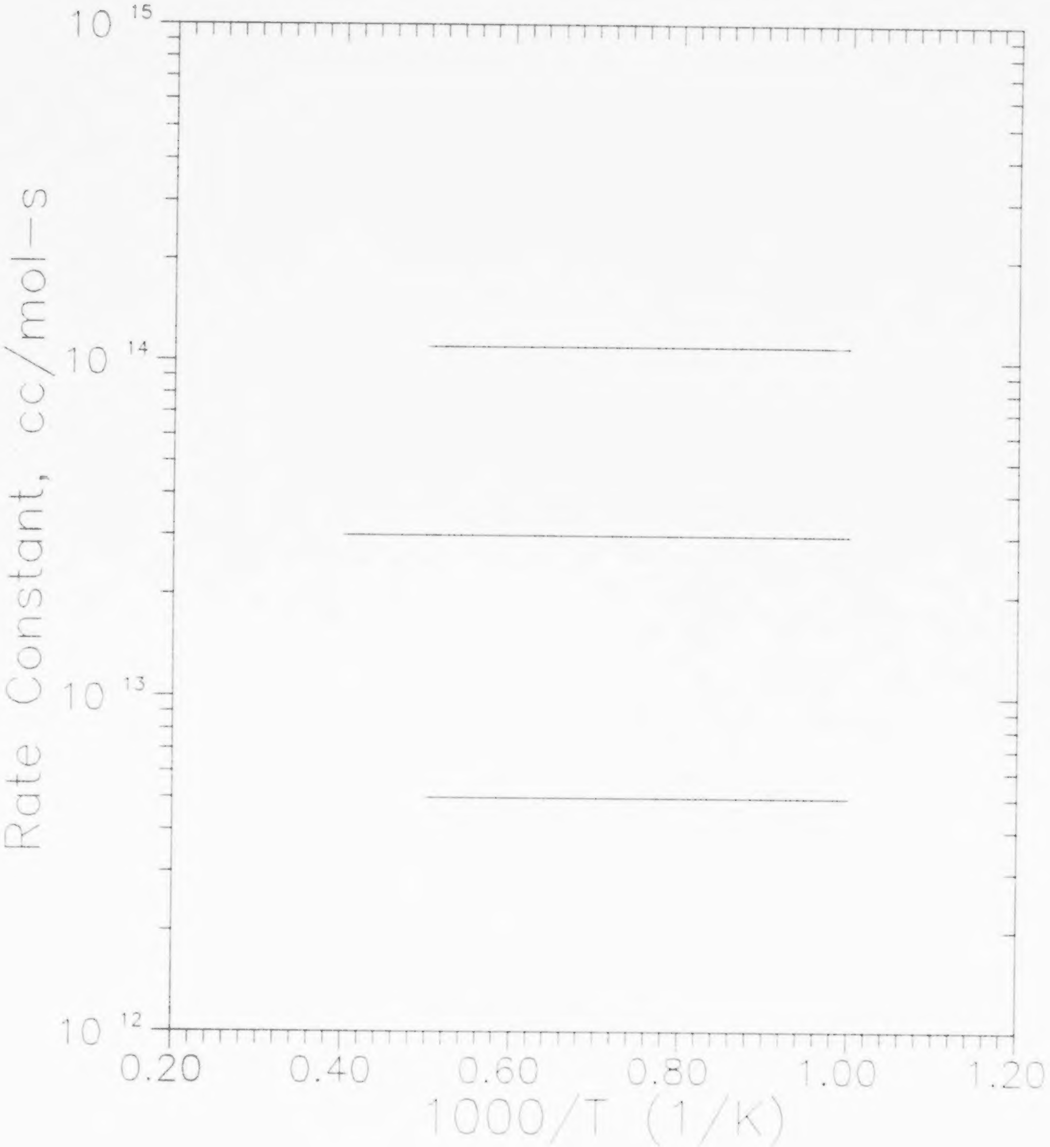
**CH2CO + H = CH3 + CO**



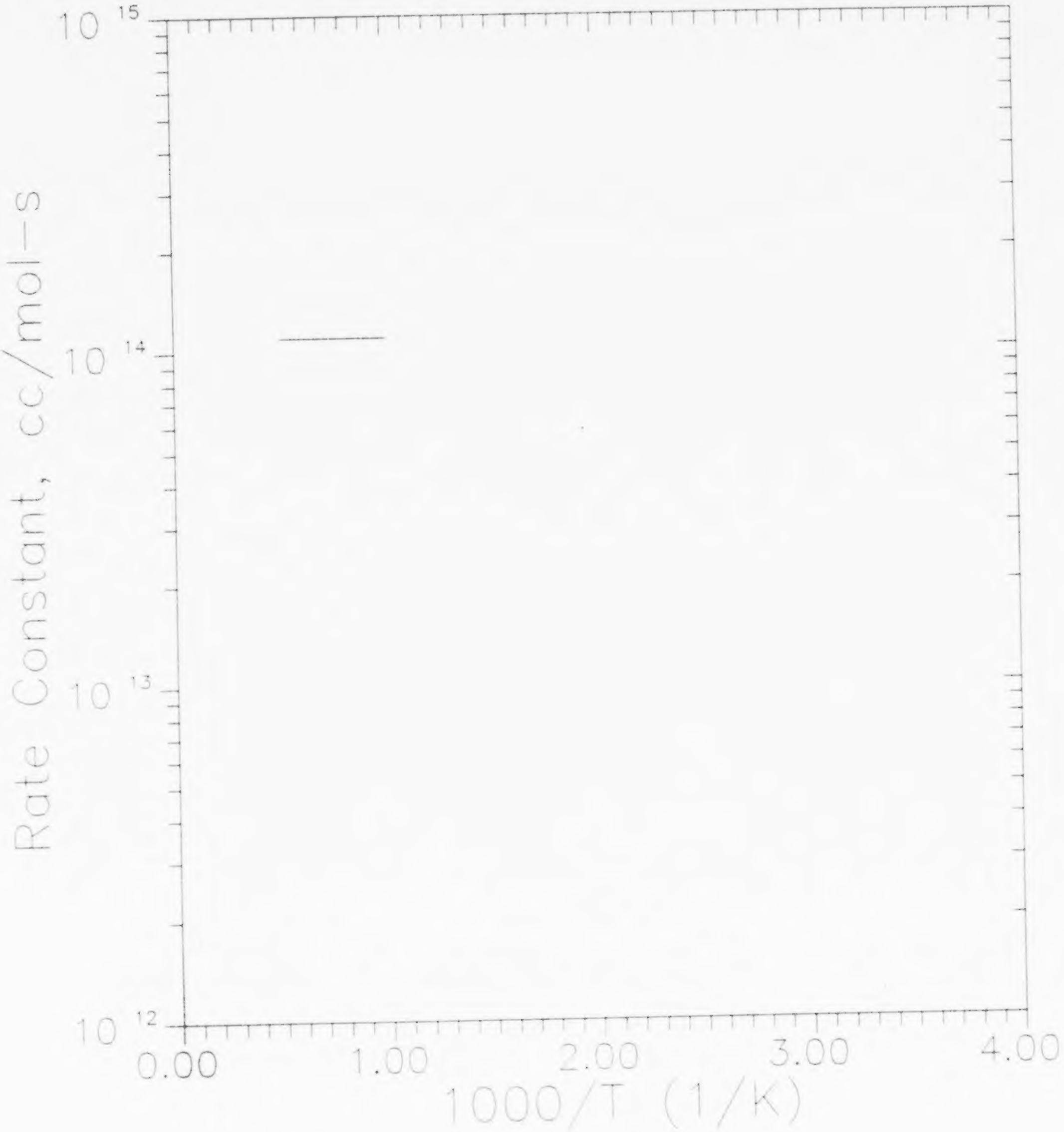
**CH2CO + HO = CH2O + CHO**



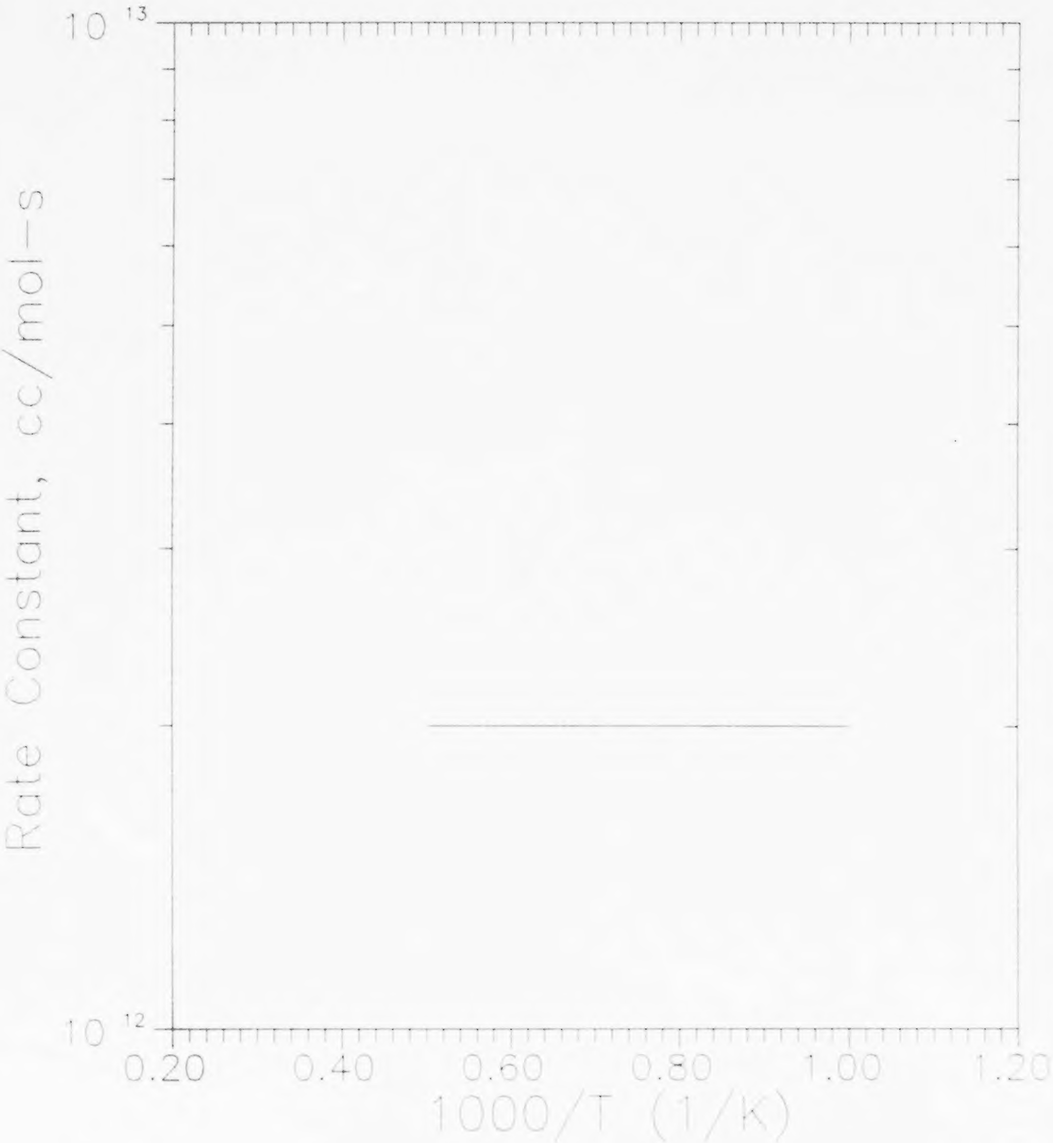
**CH2CO + HO = CHCO + H2O**


10 15
10 14
10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

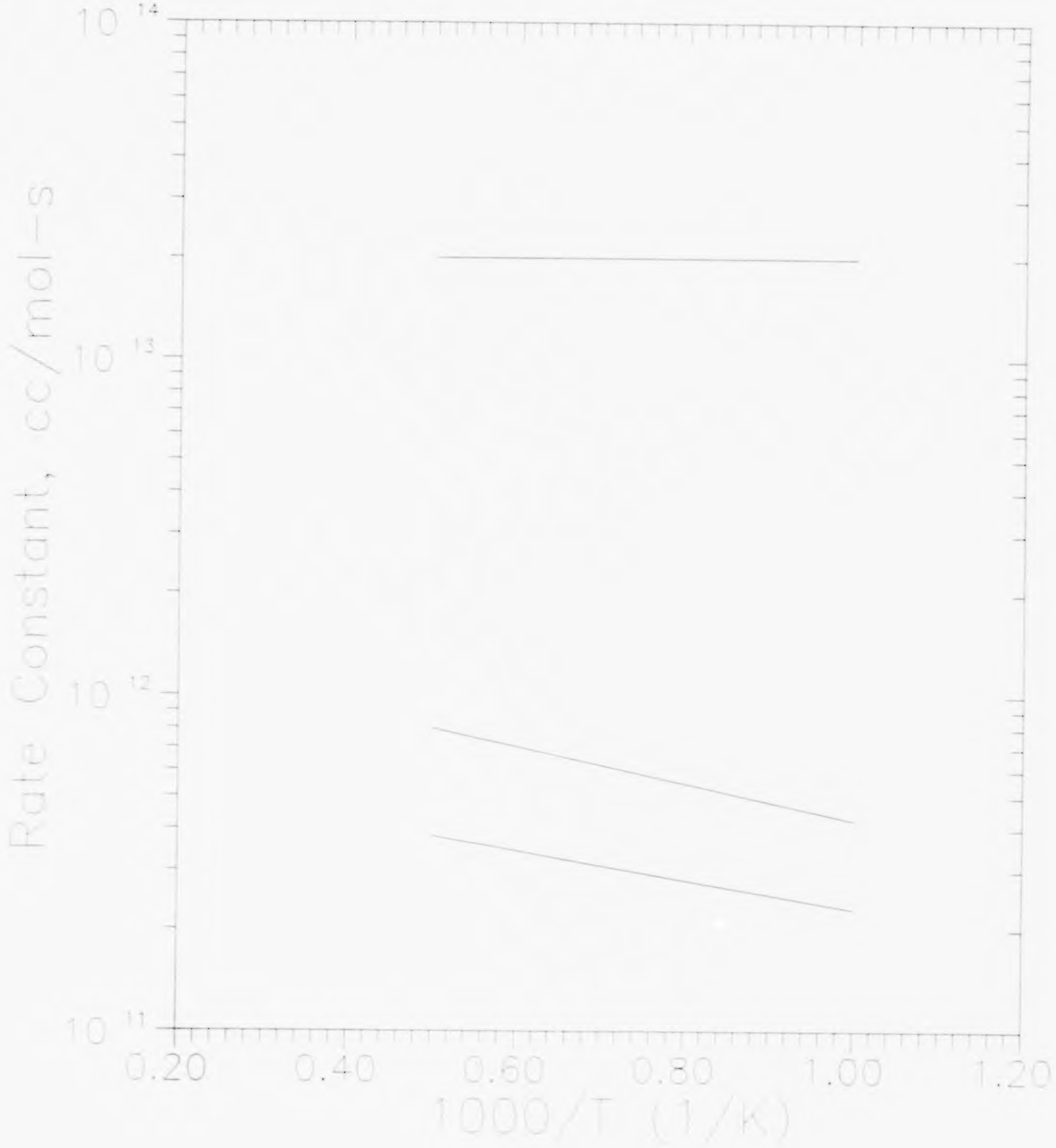
**CHCO + H = CH2 + CO**


Rate Constant, cc/mol-s
10 15
10 14
10 13
10 12
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

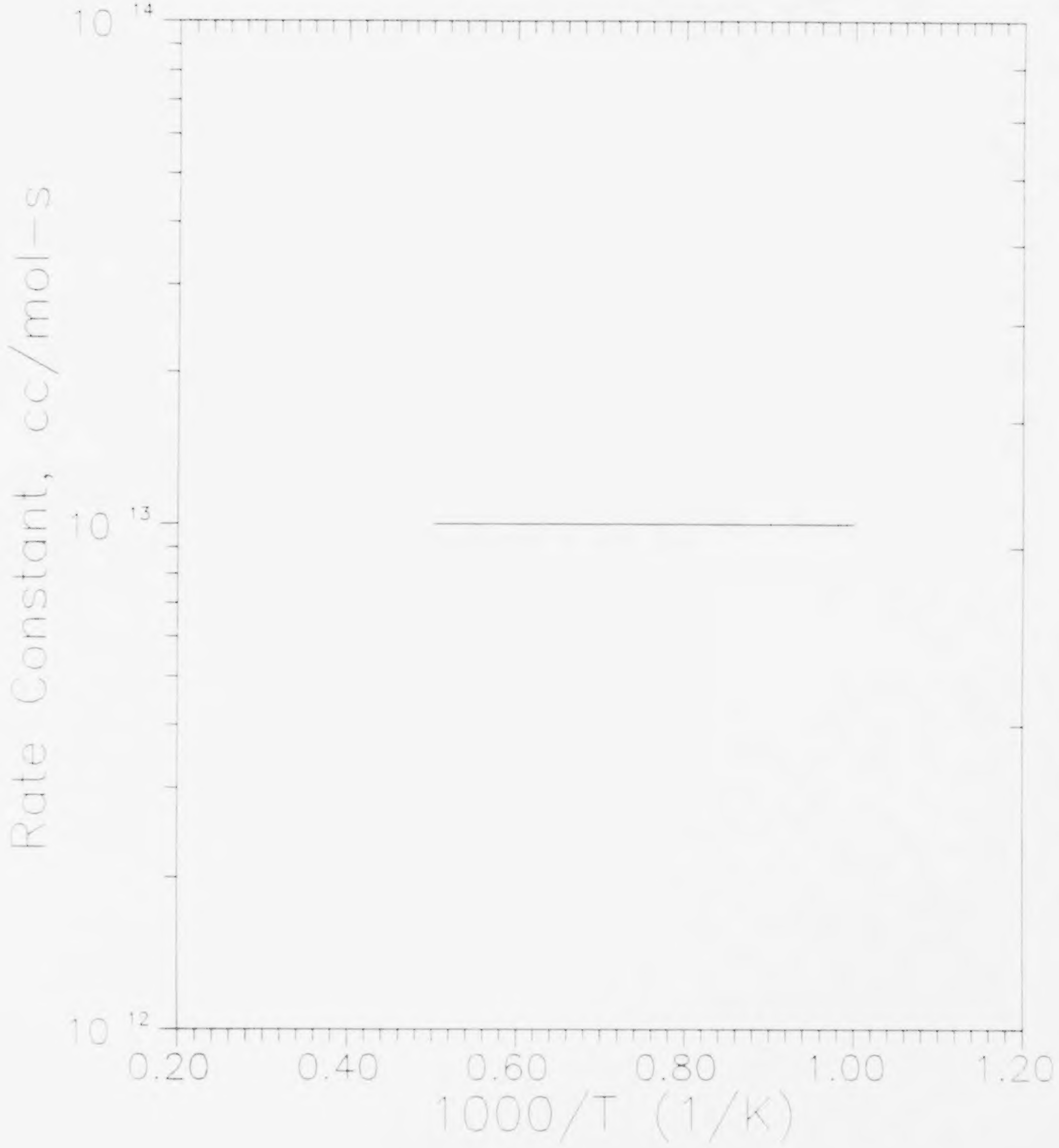
**CHCO + O = CO + CO + H**



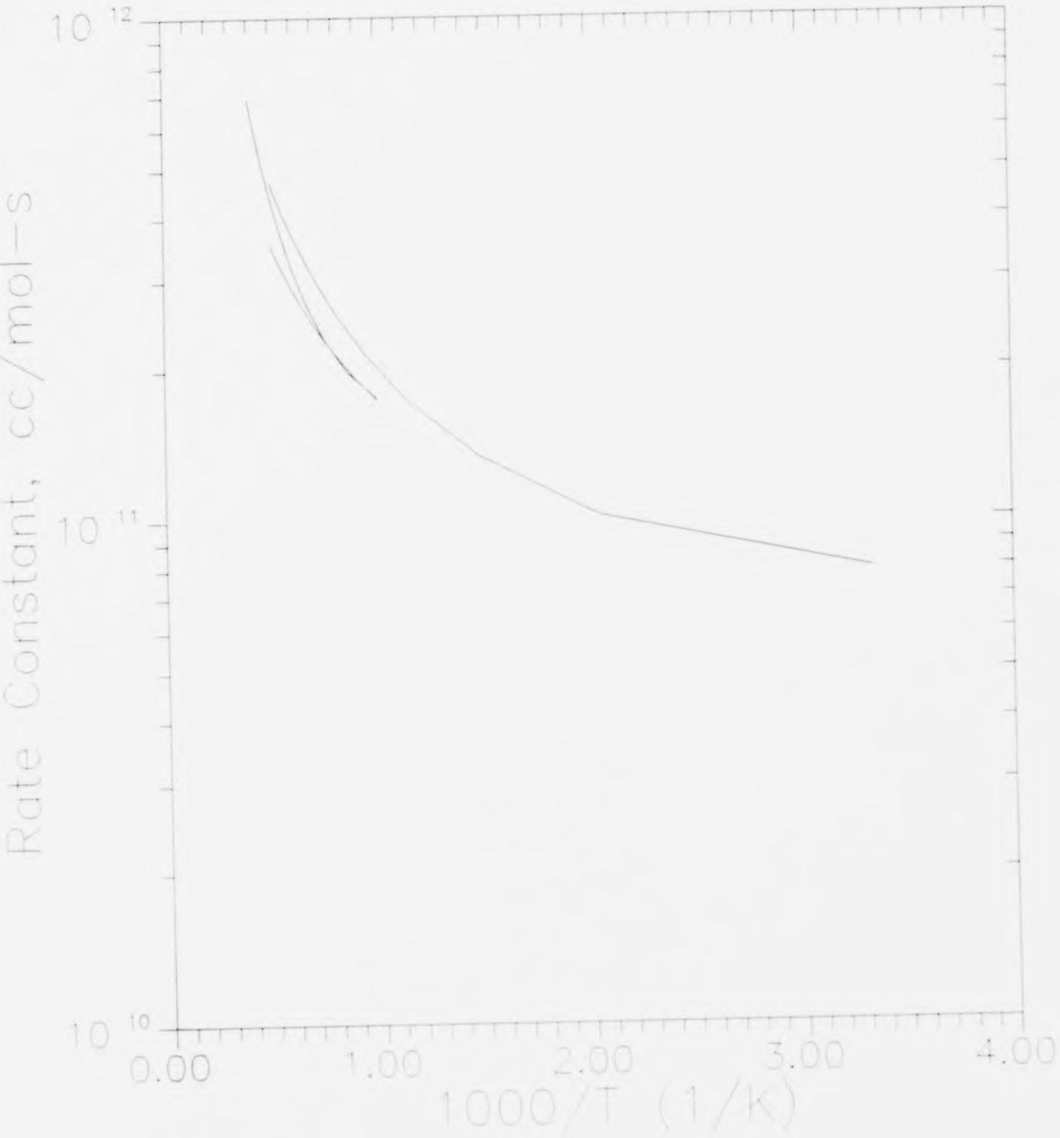
**CHCO + HO = CHO + CO + H**



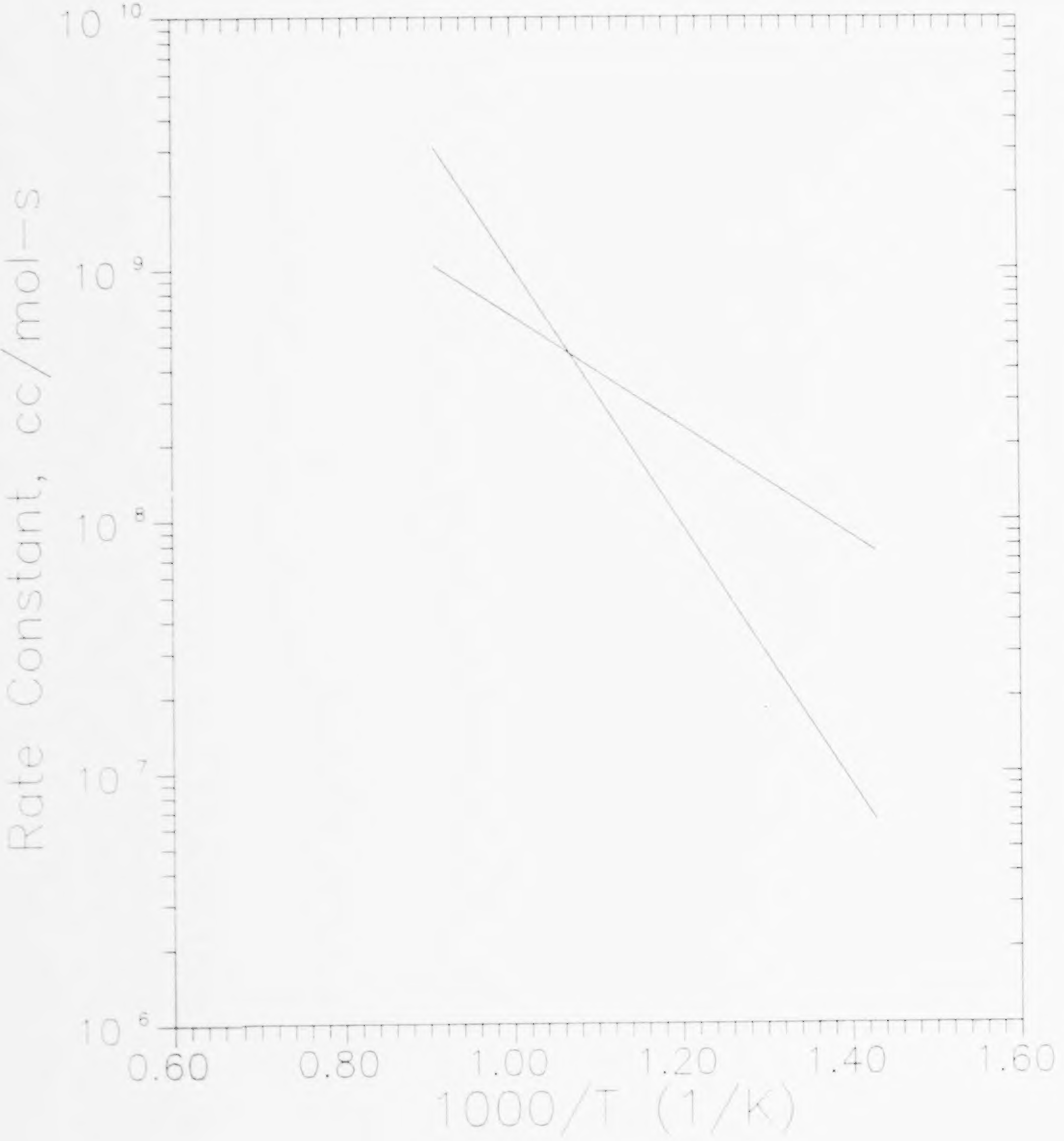
CHCO + O2 = CO + CO + HO



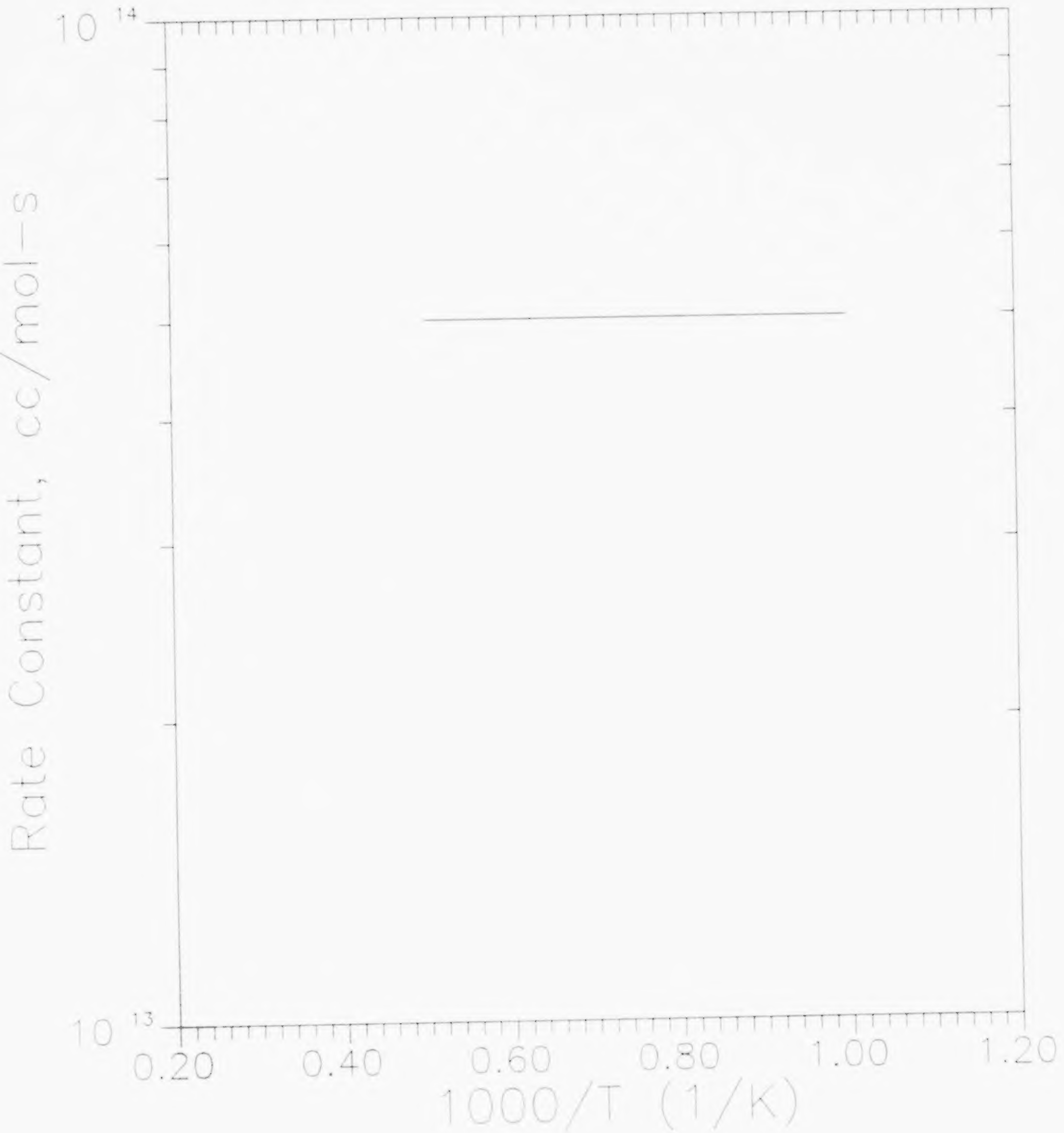
**CHCO + CHCO = C2H2 + CO + CO**


$10^{12}$
$10^{11}$
$10^{10}$
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/k)

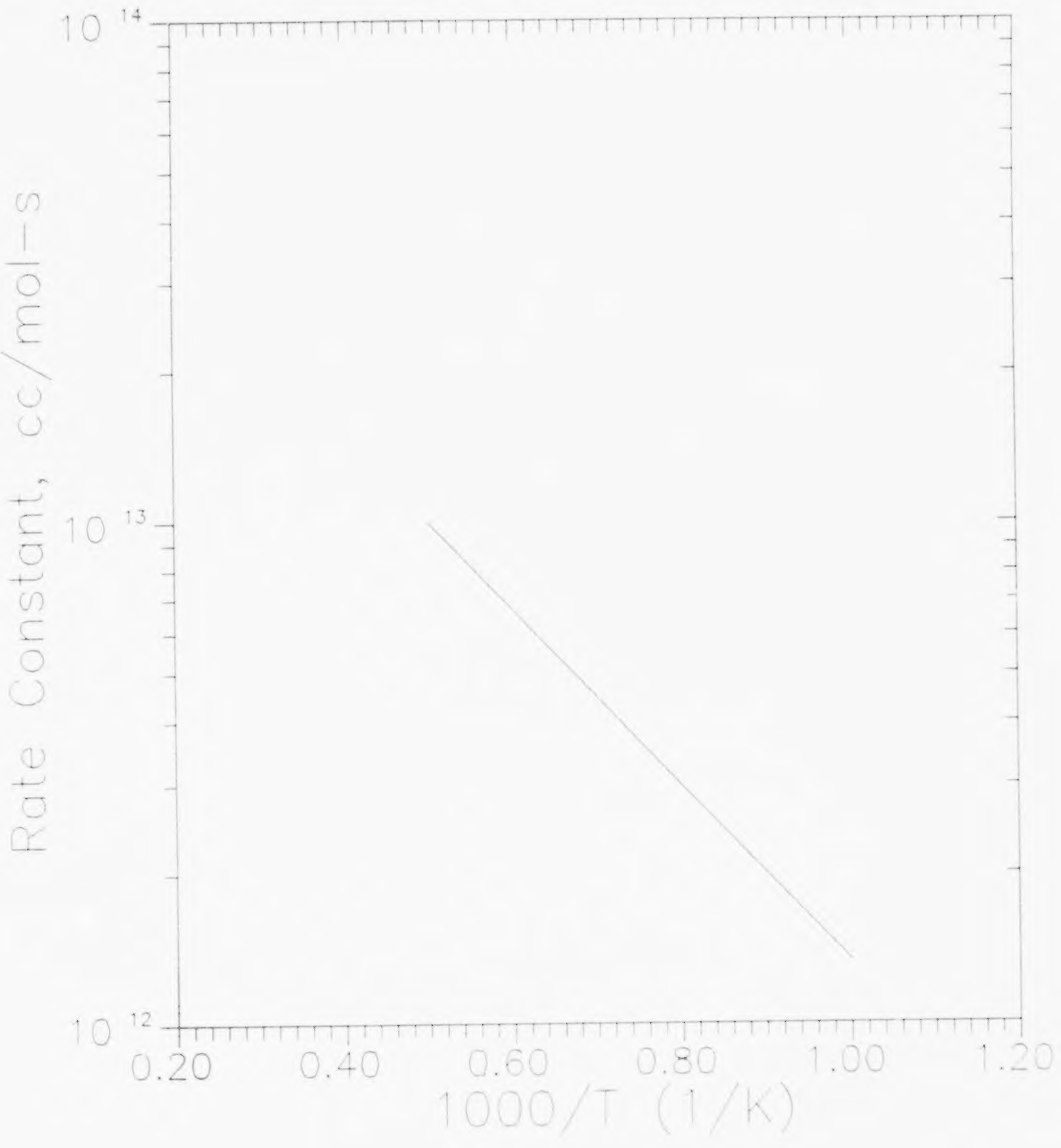
**CO + HO = CO2 + H**


Rate Constant, cc/mol-s
10^10
10^9
10^8
10^7
10^6
0.60
0.80
1.00
1.20
1.40
1.60
1000/T (1/K)

**CO + HO2 = CO2 + HO**


Rate Constant, cc/mol-s
10 14
10 13
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

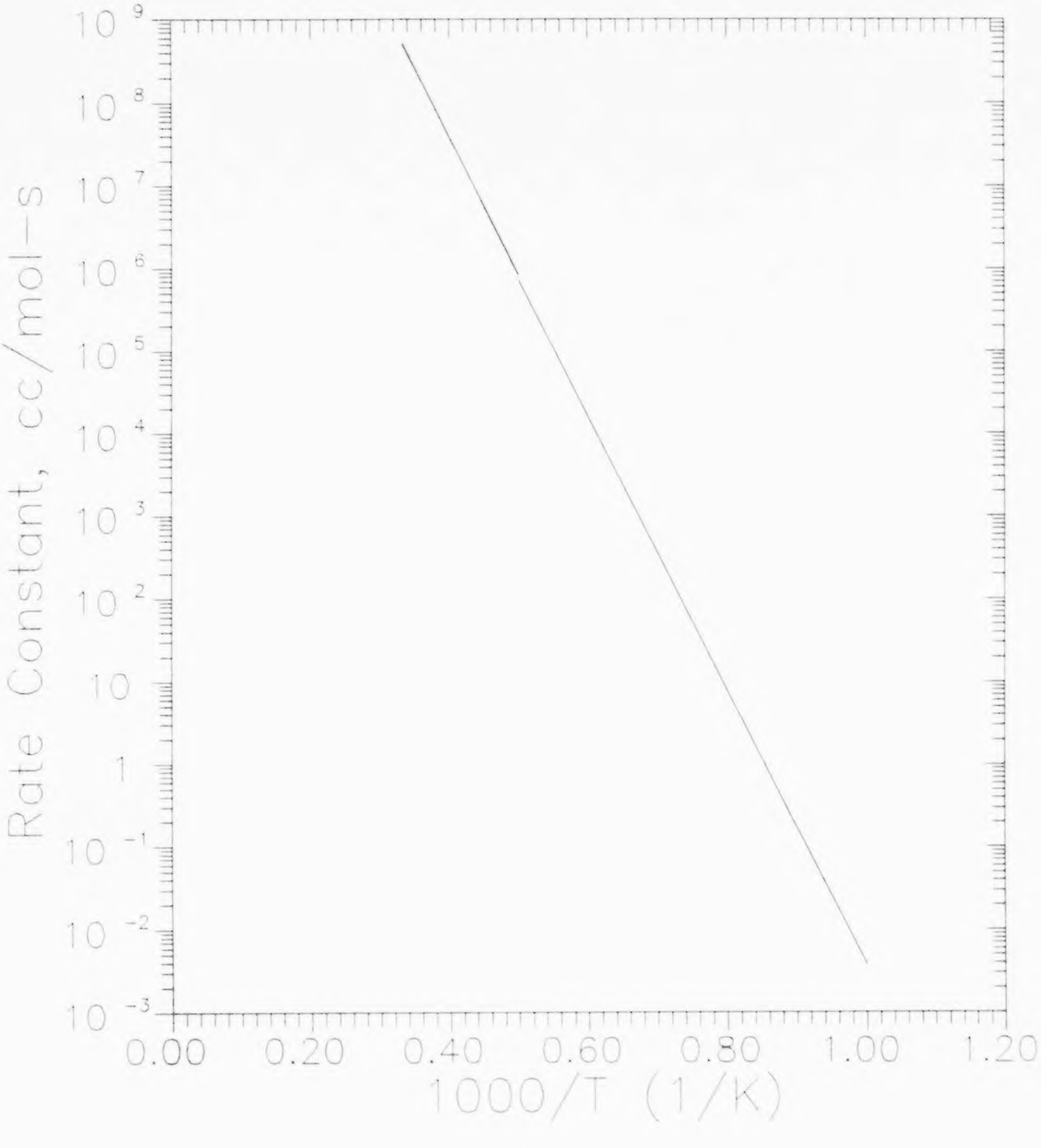
**C + HO = CO + H**



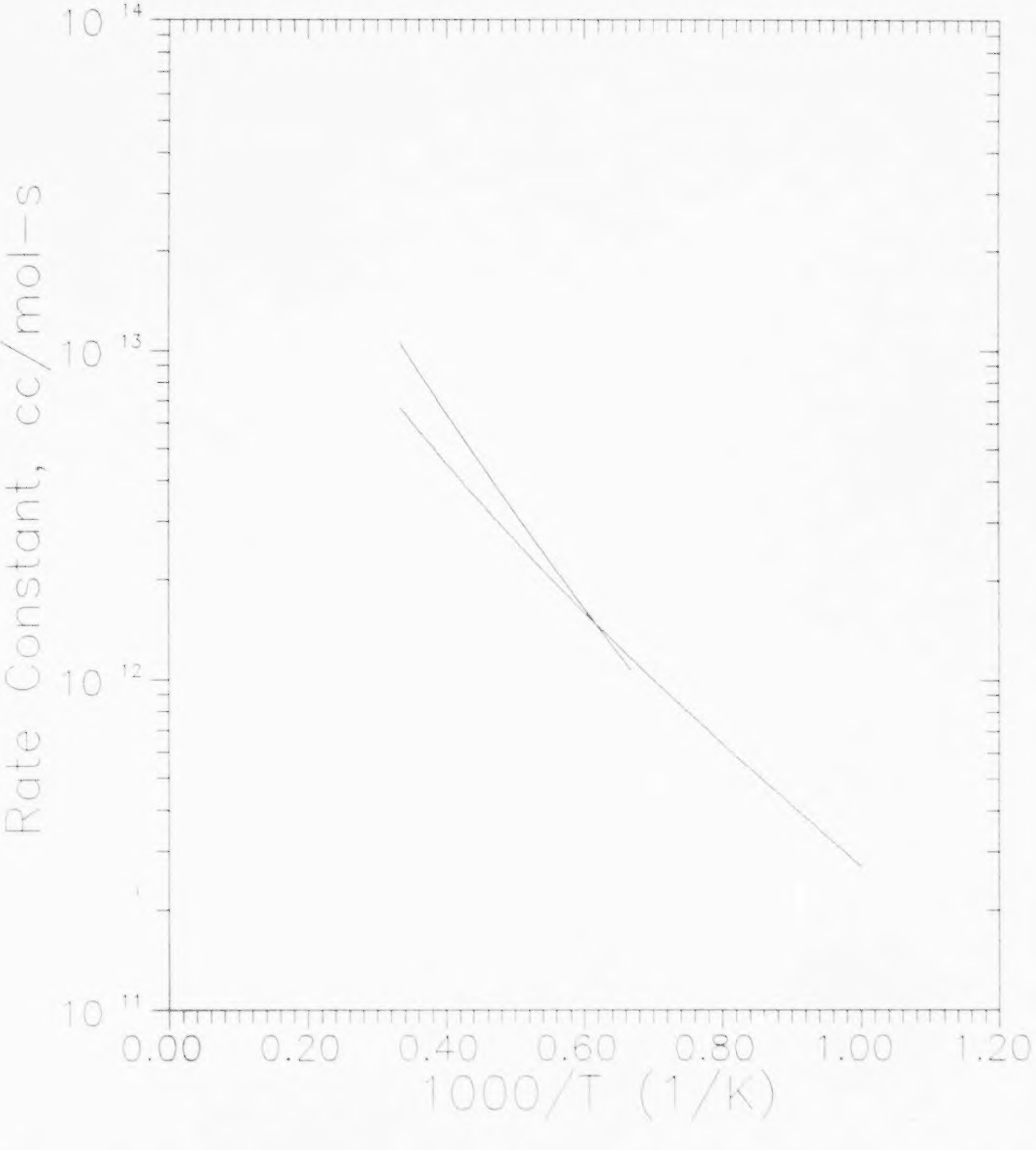
CH2CO + H = CHCO + H2

```
*----------------------------------------------------------------------------*
!  File: NOMECH.DAT                                                          !
! Saved: 08-04-88 at 11:06:22 am                                     Page  1 !
*----------------------------------------------------------------------------*

 1N2   + 1O            = 1N    + 1NO
Forward Rate Parameters:
Hanson, Salimian in comb chem          1.8E+14 0.000 76.200  2000.0  3000.0
Reverse Rate Parameters:
Glarborg, et al. 1985                  3.3E+12 0.300  0.000  2000.0  3000.0
Glarborg, et al. 1986
Seeker, et al. 1985                    3.1E+13 0.000  0.334  1000.0  2000.0

 1N    + 1O2           = 1NO   + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                  6.4E+09 1.000  6.280  1000.0  3000.0
Glarborg, et al. 1986
Seeker, et al. 1985
Reverse Rate Parameters:
Hanson, Salimian in comb chem          3.8E+09 1.000 41.350  1500.0  3000.0

 1NO   + 1N2O          = 1N2   + NO2
Forward Rate Parameters:
Seeker, et al. 1985                    2.0E+14 0.000  5.000  1000.0  2000.0

 1NO   + 1O    + 1M    = 1NO2  + 1M
Forward Rate Parameters:
Seeker, et al. 1985                    1.0E+21-1.860  0.000  1000.0  2000.0
Reverse Rate Parameters:
Glarborg, et al. 1985                  1.1E+16 0.000 66.000  1000.0  2000.0
Glarborg, et al. 1986
Lyon, 1987
Hanson, Salimian in comb chem

 1NO2  + 1O            = 1NO   + 1O2
Forward Rate Parameters:
Glarborg, et al. 1985                  1.0E+13 0.000  0.600  1000.0  2000.0
Glarborg, et al. 1986
Lyon, 1987
Hanson, Salimian in comb chem
Seeker, et al. 1985

 1N2O  + 1M            = 1N2   + 1O    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                  1.6E+14 0.000 51.600  1810.0  3360.0
Glarborg, et al. 1986
Seeker, et al. 1985                    1.4E+14 0.000 51.280  1810.0  3360.0
Hanson, Salimian in comb chem          6.92E23-2.500 64.960  1500.0  3000.0

 1N2O  + 1O            = 1NO   + 1NO
Forward Rate Parameters:
Glarborg, et al. 1985                  1.0E+14 0.000 28.200  1200.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                    3.09E13 0.000 21.800  2380.0  3000.0
Hanson, Salimian in comb chem          6.92E13 0.000 26.610  1200.0  3000.0

 1N2O  + 1O            = 1N2   + 1O2
Forward Rate Parameters:
Glarborg, et al. 1985                  1.0E+14 0.000 28.200  1200.0  3000.0
Glarborg, et al. 1986
```

```
Hanson, Salimian in comb chem
Seeker, et al. 1985                         6.2E+13 0.000 24.540  1680.0  2000.0
```

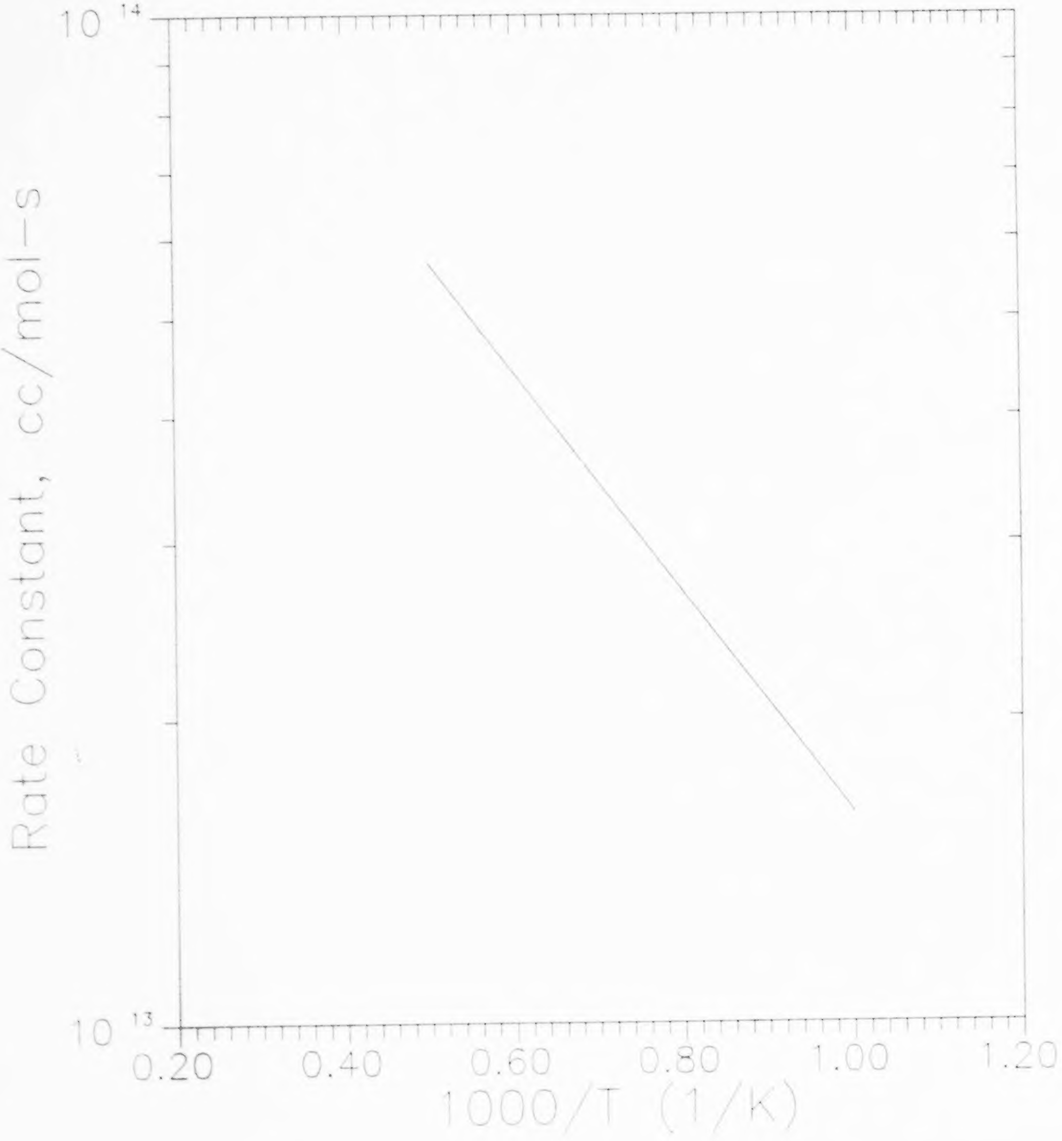

Rate Constant, cc/mol-s
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
$10^{5}$
$10^{4}$
$10^{3}$
$10^{2}$
10
1
$10^{-1}$
$10^{-2}$
$10^{-3}$
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**N2 + O = N + NO**

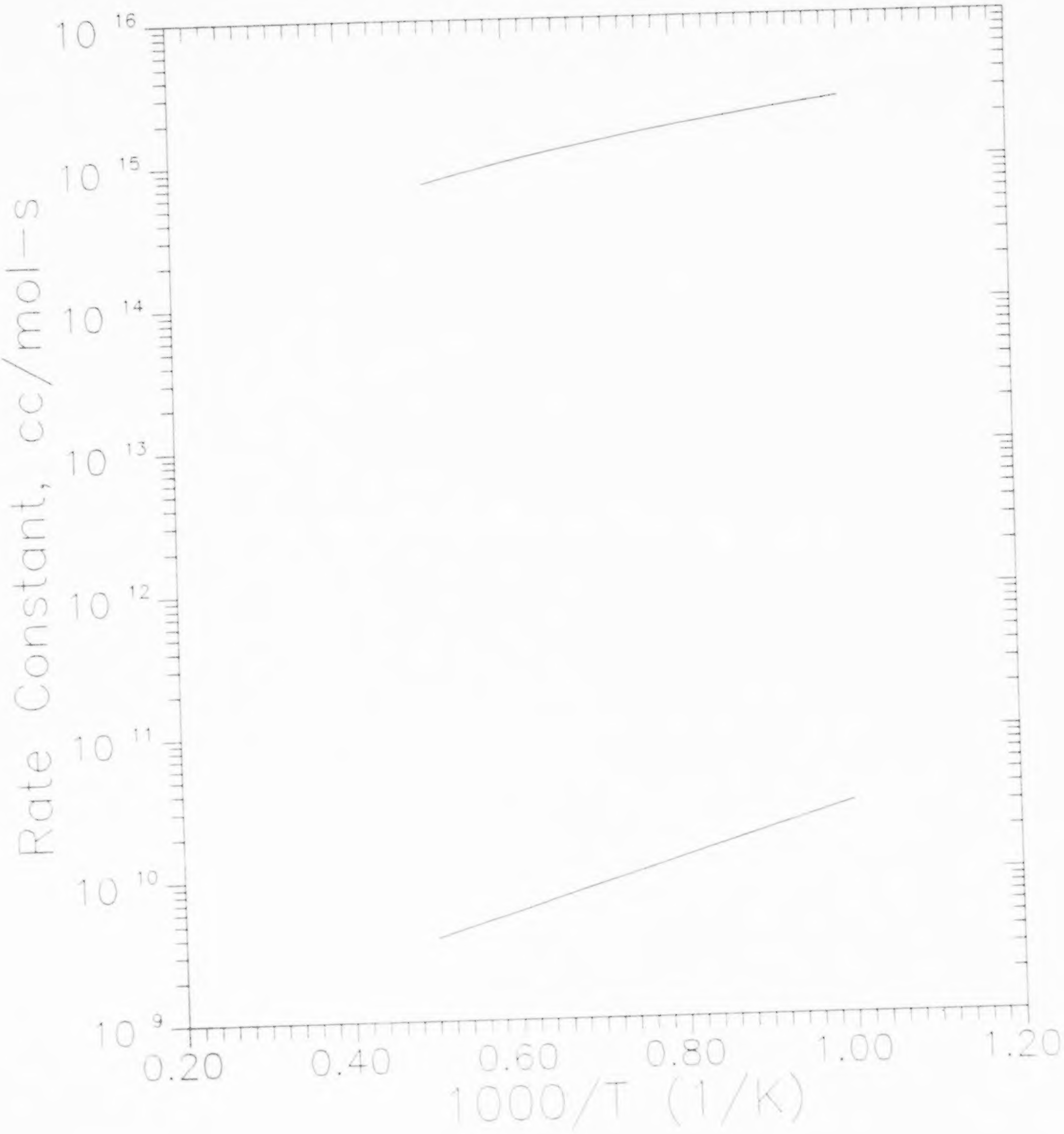


Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**N + O2 = NO + O**


10 14
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NO + N2O = N2 + O2**



Rate Constant, cc/mol-s
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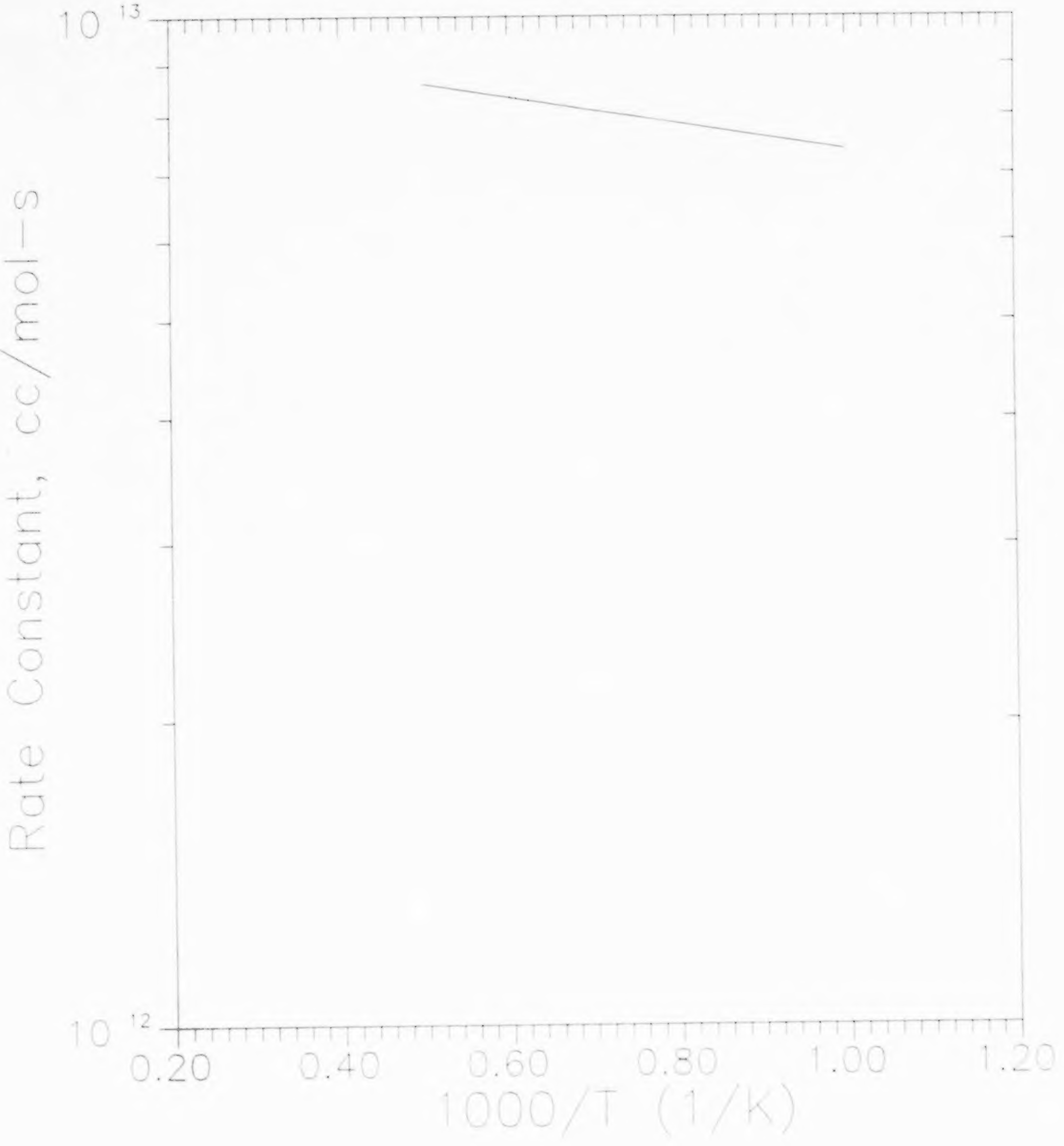
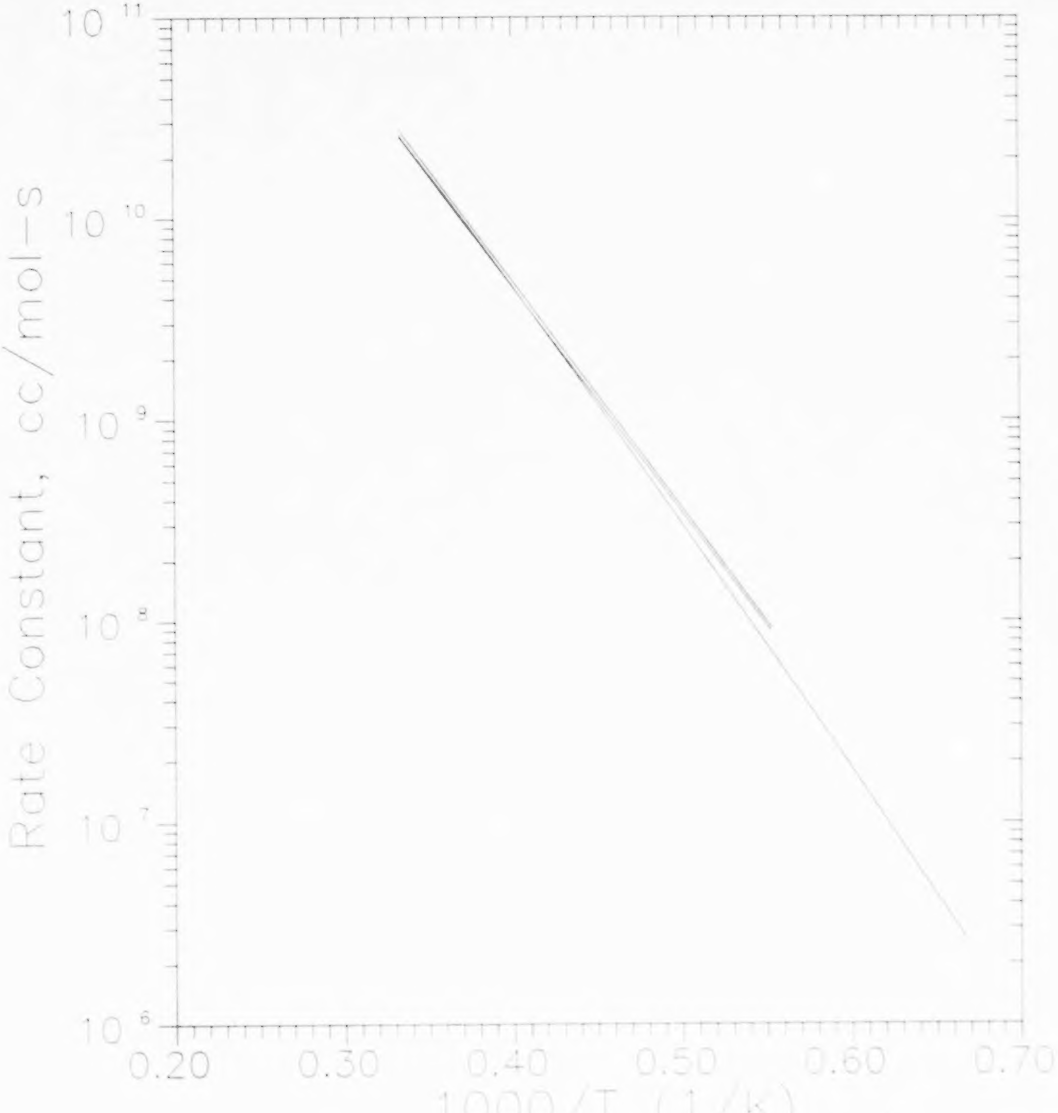
$10^{15}$
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NO + O + M = NO2 + M**

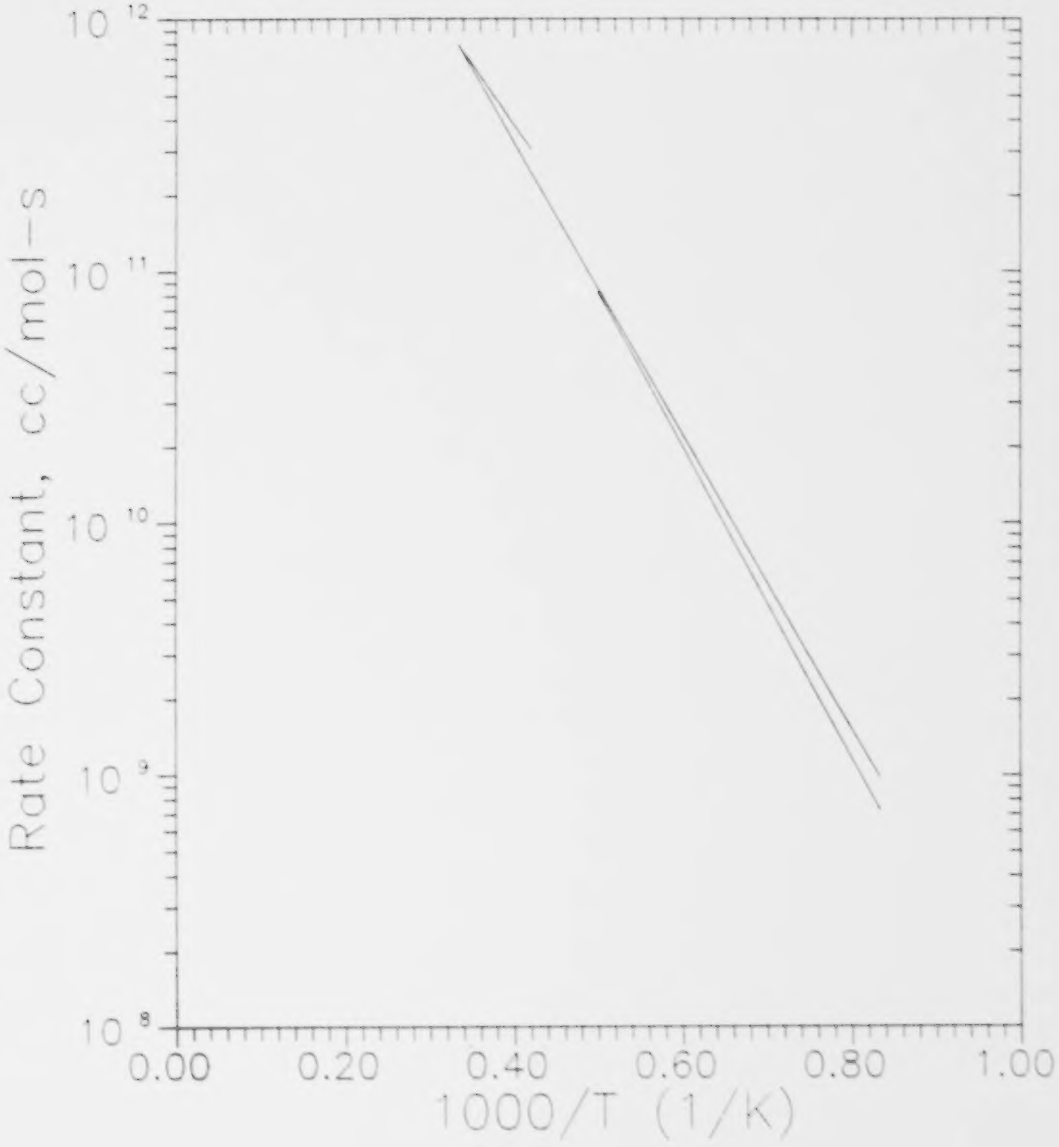

10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NO2 + O = NO + O2**

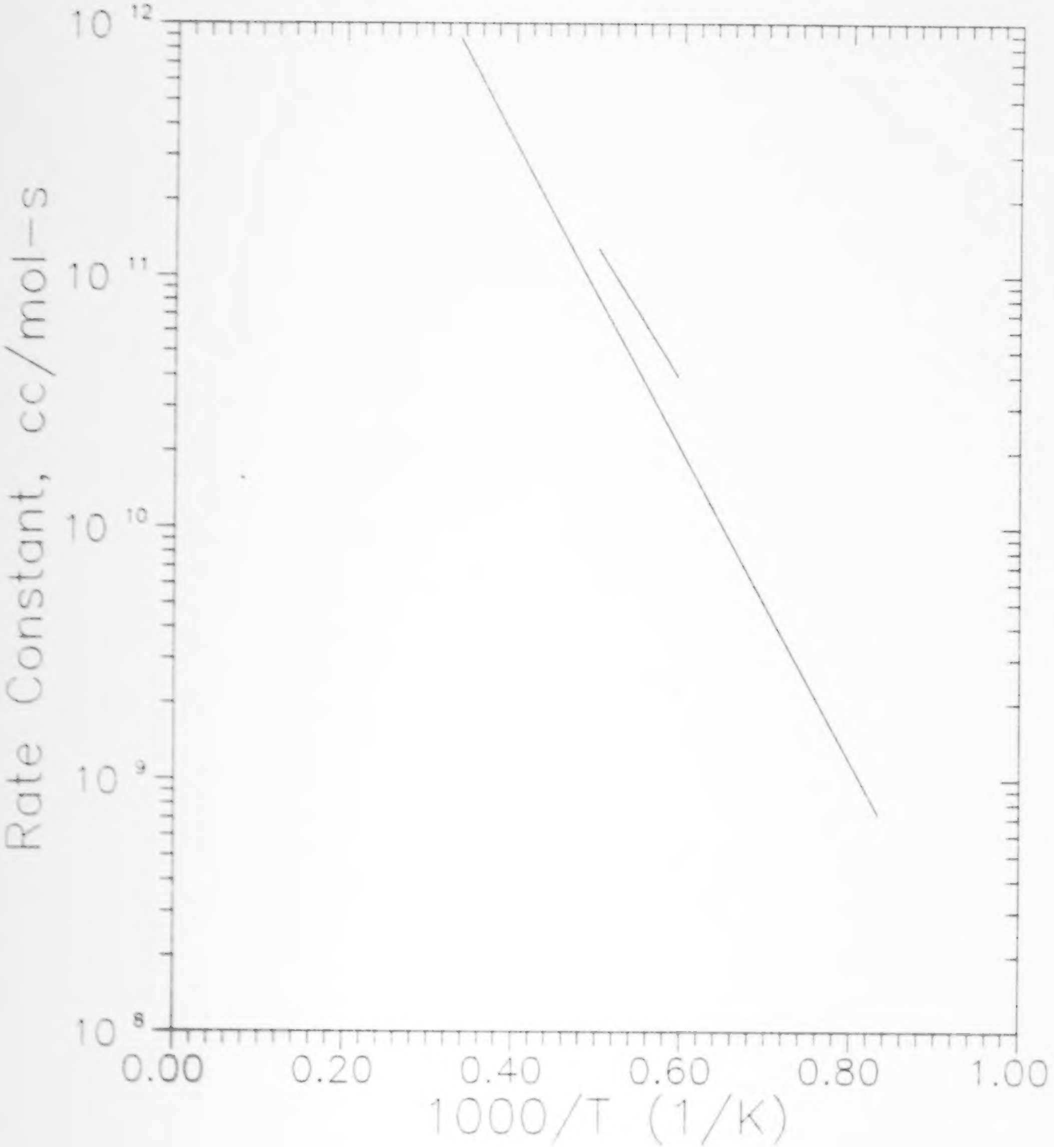


Rate Constant, cc/mol-s
$10^{11}$
$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
0.20
0.30
0.40
0.50
0.60
0.70
1000/T (1/K)

**N2O + M = N2 + O + M**


Rate Constant, cc/mol-s
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
$10^{8}$
0.00
0.20
0.40
0.60
0.80
1.00
1000/T (1/K)

**N2O + O = NO + NO**



10^12
10^11
10^10
10^9
10^8
Rate Constant, cc/mol-s
0.00
0.20
0.40
0.60
0.80
1.00
1000/T (1/K)

**N2O + O = N2 + O2**

```
*---------------------------------------------------------------------------*
| File: NHMECH.DAT                                                           |
| Saved: 08-04-88 at 11:06:10 am                                    Page  1 |
*---------------------------------------------------------------------------*

 1N2   + 1M           = 1N    + 1N    + 1M
Forward Rate Parameters:
Seeker, et al. 1985                   3.7E+21-1.600225.000  1000.0  2000.0

 1NH3  + 1M           = 1NH2  + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                 1.4E+16 0.000 90.600  2000.0  3000.0
Glarborg, et al. 1986
Seeker, et al. 1985                   2.5E+16 0.000 93.700  1740.0  3450.0
Hanson, Salimian in comb chem
Lyon, 1987                            4.8E+16 0.000 93.900  2200.0  3300.0

 1NH3  + 1M           = 1NH   + 1H2   + 1M
Forward Rate Parameters:
Seeker, et al. 1985                   2.5E+14 0.000 93.800  2200.0  3000.0
Hanson, Salimian in comb chem         6.3E+14 0.000 93.300  2200.0  3000.0


 1NH3  + 1H           = 1NH2  + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                 6.9E+13 0.000 13.216  1000.0  2000.0
Glarborg, et al. 1986                 7.0E+06 2.390 10.171  1000.0  2000.0
Seeker, et al. 1985                   3.6E+10 0.750 13.790  1000.0  2000.0
Lyon, 1987                            2.5E+13 0.000 17.100  1500.0  2150.0
Hanson, Salimian in comb chem         1.3E+14 0.000 21.500  1500.0  2500.0

 1NH3  + 1N           = 1NH   + 1NH2
Forward Rate Parameters:
Seeker, et al. 1985                   1.0E+11 0.500 31.640  1000.0  2000.0

 1NH2  + 1M           = 1NH   + 1H    + 1M
Forward Rate Parameters:
Hanson, Salimian in comb chem         3.2E+23-2.000 91.400  1000.0  2000.0
Reverse Rate Parameters:
Seeker, et al. 1985                   2.0E+16-0.500  0.000  1000.0  2000.0

 1NH2  + 1H           = 1NH   + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                 6.9E+13 0.000  3.650  2800.0  2801.0
Glarborg, et al. 1986
Seeker, et al. 1985                   5.0E+11 0.500  7.570  1450.0  3000.0
Hanson, Salimian in comb chem         1.9E+13 0.000  0.000  2400.0  3000.0

 1NH2  + 1HN2         = 1N2   + 1NH3
Forward Rate Parameters:
Lyon, 1987                            1.0E+13 0.000  0.000  1000.0  2000.0
Hanson, Salimian in comb chem

 1NH2  + 1NH          = 1N2H2 + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                 5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Hanson, Salimian in comb chem         3.2E+13 0.000  1.000  1000.0  2000.0

 1NH2  + 1N           = 1N2   + 1H    + 1H
```

```
*---------------------------------------------------------------------------*
|  File: NHMECH.DAT                                                         |
| Saved: 08-04-88 at 11:06:10 am                                   Page  2  |
*---------------------------------------------------------------------------*

Forward Rate Parameters:
Glarborg, et al. 1985                   7.2E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1NH2  + 1N           = 1NH   + 1NH
Forward Rate Parameters:
Seeker, et al. 1985                     2.0E+11 0.500 22.160  1000.0  2000.0
Reverse Rate Parameters:
Hanson, Salimian in comb chem           2.0E+11 0.500  2.000  1000.0  2000.0

 1NH2  + 1NH2         = 1NH3  + 1NH
Forward Rate Parameters:
Seeker, et al. 1985                     1.2E+11 0.500  5.640  1000.0  2000.0
Hanson, Salimian in comb chem           6.3E+12 0.000  9.930  1000.0  2000.0

 1NH2  + 1NH2         = 1N2   + 1H2   + 1H2
Forward Rate Parameters:
Seeker, et al. 1985                     4.0E+13 0.000 12.000  1000.0  2000.0

 1NH   + 1N           = 1N2   + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                     6.3E+11 0.500  0.000  1000.0  2000.0
Hanson, Salimian in comb chem

 1NH   + 1H           = 1N    + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                   3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                     6.3E+11 0.500  8.000  1000.0  2000.0
Hanson, Salimian in comb chem           5.0E+13 0.000  1.990  1000.0  2000.0

 1NH   + 1NH          = 1N2   + 1H2
Forward Rate Parameters:
Seeker, et al. 1985                     3.6E+11 0.550  1.900  1000.0  2000.0

 1NH   + 1M           = 1N    + 1H    + 1M
Forward Rate Parameters:
Hanson, Salimian in comb chem           3.2E+21-2.000 83.400  1000.0  2000.0
Reverse Rate Parameters:
Seeker, et al. 1985                     3.0E+16-0.500  0.000  1000.0  2000.0

 1HN2  + 1M           = 1N2   + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                   2.0E+14 0.000 20.000  1000.0  2000.0
Glarborg, et al. 1986
Hanson, Salimian in comb chem
Lyon, 1987                              2.0E+14 0.000 30.000  1000.0  2000.0

 1HN2  + 1H           = 1N2   + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                   3.7E+13 0.000  3.000  1000.0  2000.0
Glarborg, et al. 1986
Hanson, Salimian in comb chem           4.0E+13 0.000  3.000  1000.0  2000.0
```

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*--------------------------------------------------------------------------*
!  File: NHMECH.DAT                                                        !
! Saved: 08-04-88 at 11:06:10 am                                  Page  3 !
*--------------------------------------------------------------------------*


 1N2H2 + 1M            = 1HN2  + 1H    + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                 5.0E+16 0.000 50.000  1000.0  2000.0
Glarborg, et al. 1986
Hanson, Salimian in comb chem         1.0E+16 0.000 49.600  1000.0  2000.0

 1N2H2 + 1H            = 1HN2  + 1H2
Forward Rate Parameters:
Glarborg, et al. 1985                 5.0E+13 0.000  1.000  1000.0  2000.0
Glarborg, et al. 1986
Hanson, Salimian in comb chem         1.0E+13 0.000  1.000  1000.0  2000.0
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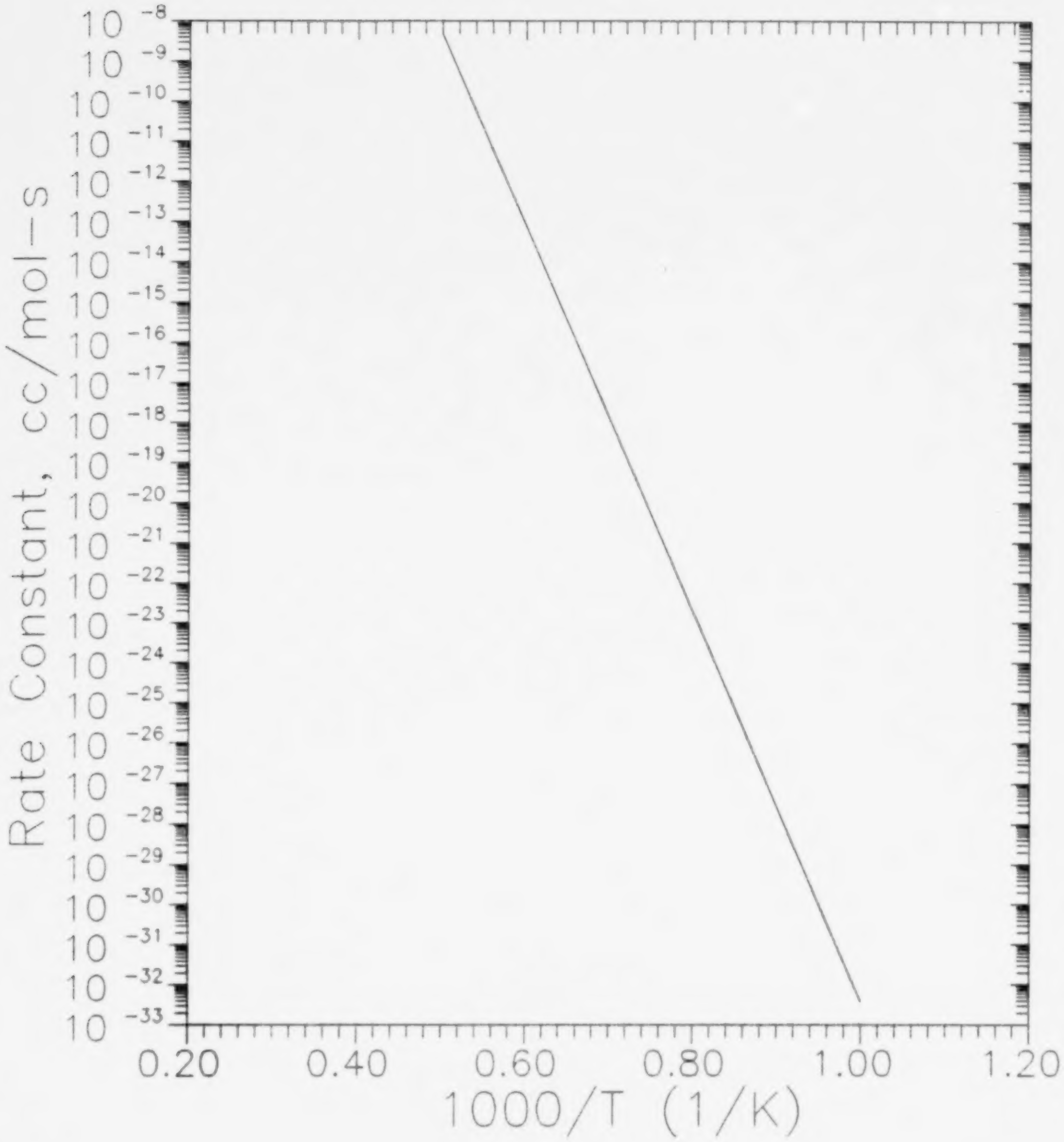
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10 -9
10 -10
10 -11
10 -12
10 -13
10 -14
10 -15
10 -16
10 -17
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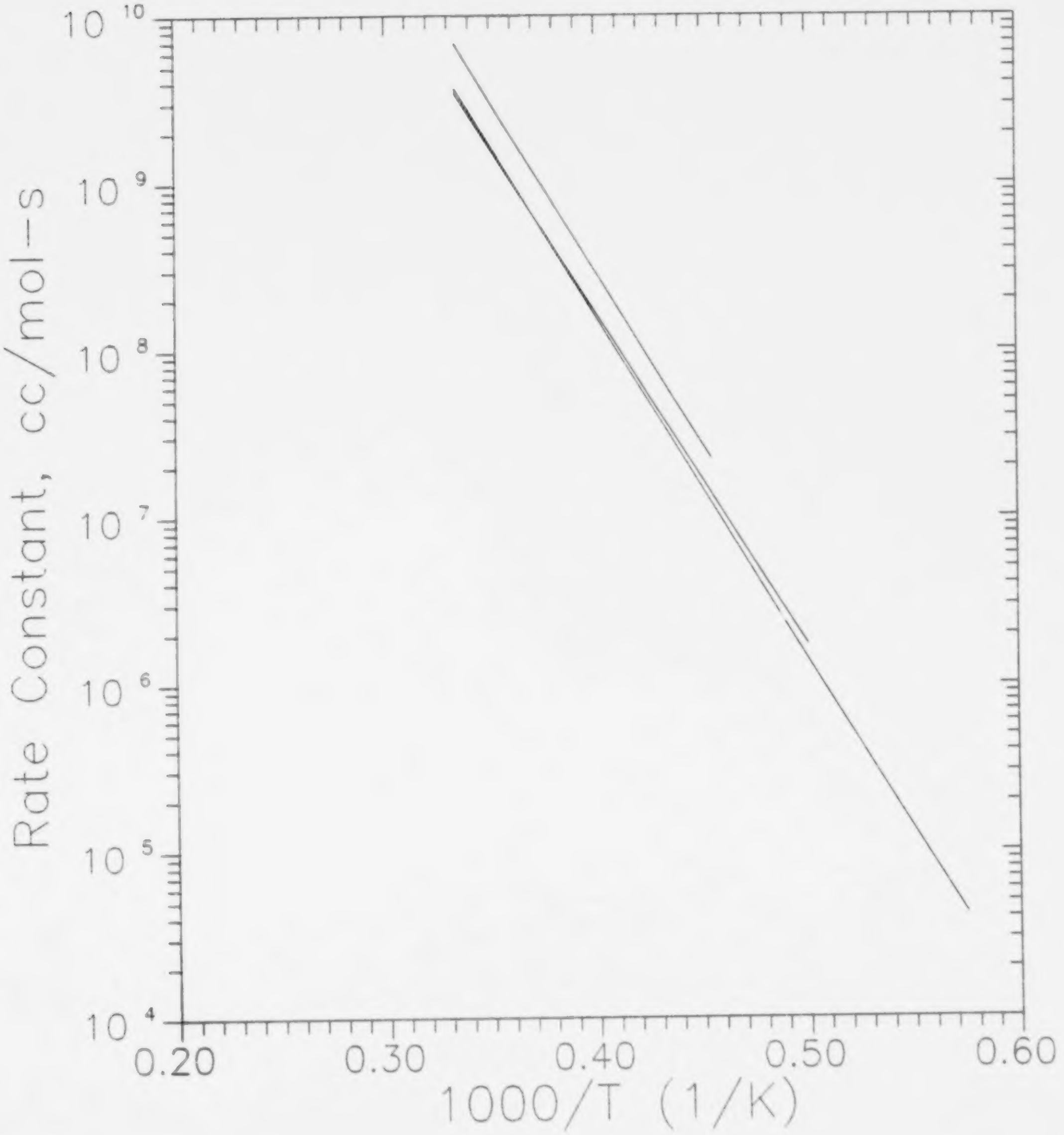
10 -19
10 -20
10 -21
10 -22
10 -23
10 -24
10 -25
10 -26
10 -27
10 -28
10 -29
10 -30
10 -31
10 -32
10 -33
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**N2 + M = N + N + M**


10 ^10
10 ^9
10 ^8
10 ^7
10 ^6
10 ^5
10 ^4
Rate Constant, cc/mol-s
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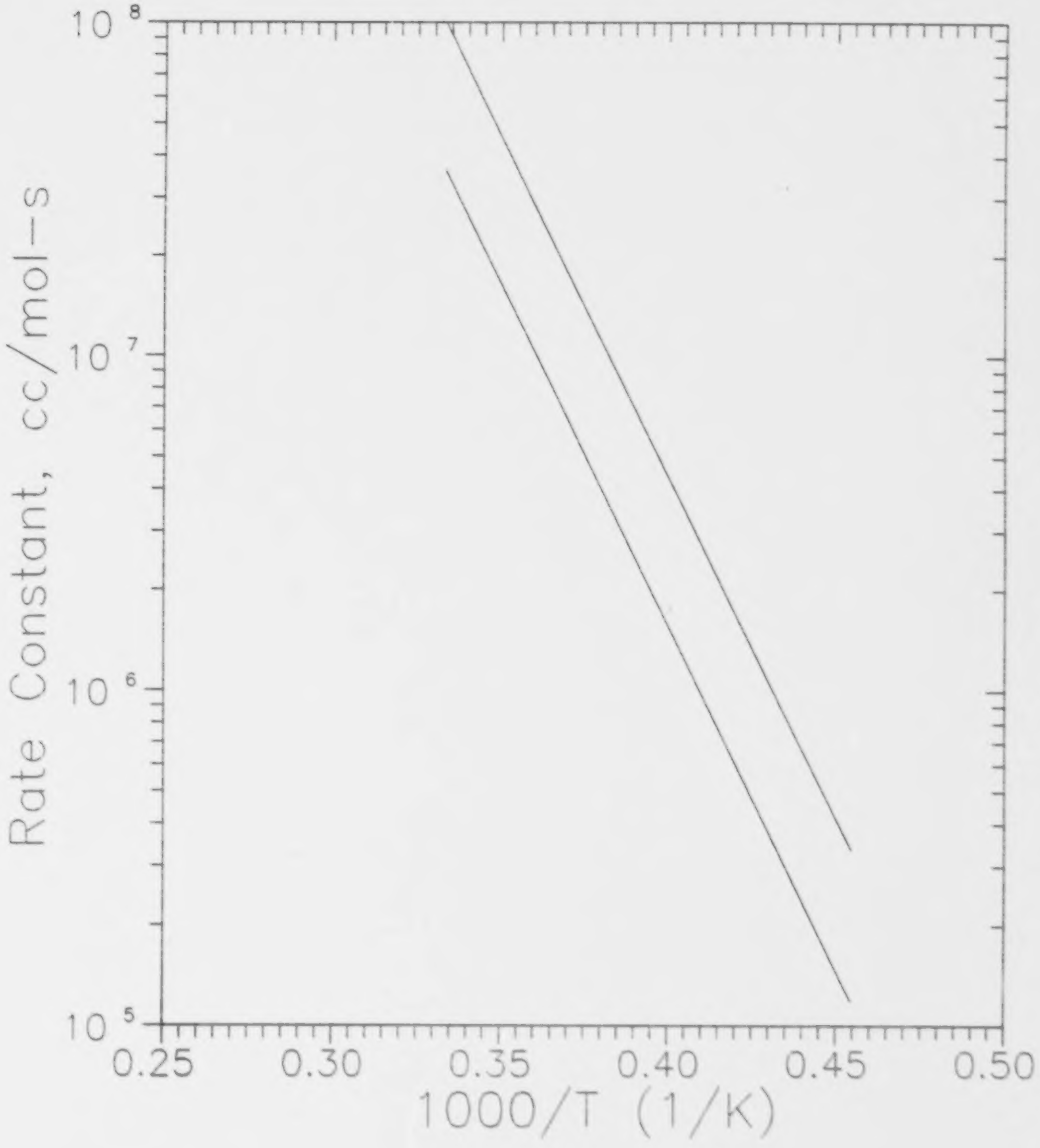
0.30
0.40
0.50
0.60
1000/T (1/K)

**NH3 + M = NH2 + H + M**



Rate Constant, cc/mol-s
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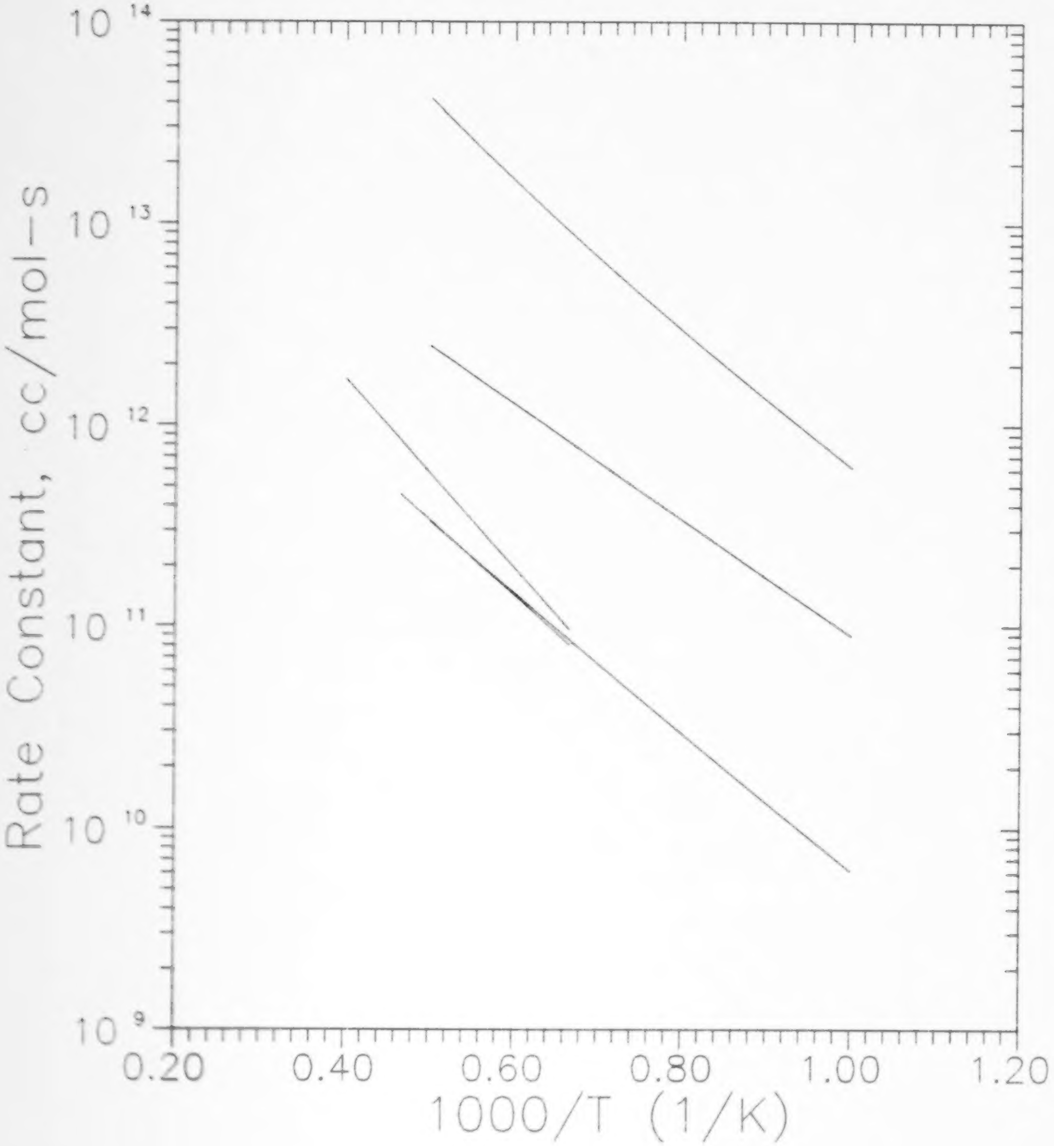
10^7
10^6
10^5
0.25
0.30
0.35
0.40
0.45
0.50
1000/T (1/K)

**NH3 + M = NH + H2 + M**



Rate Constant, cc/mol-s
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10 13
10 12
10 11
10 10
10 9
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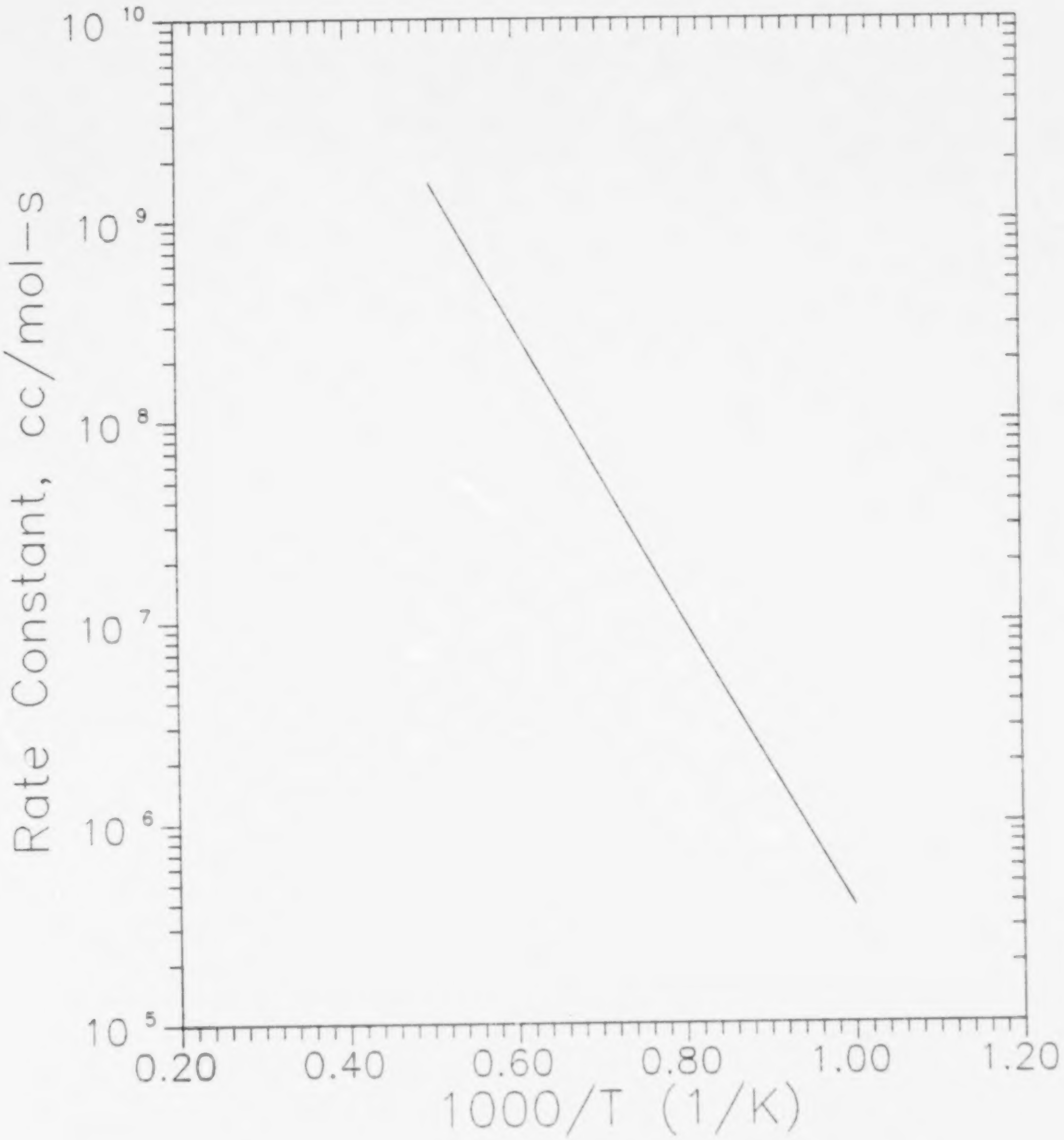
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH3 + H = NH2 + H2**


10 10
10 9
10 8
10 7
10 6
10 5
Rate Constant, cc/mol-s
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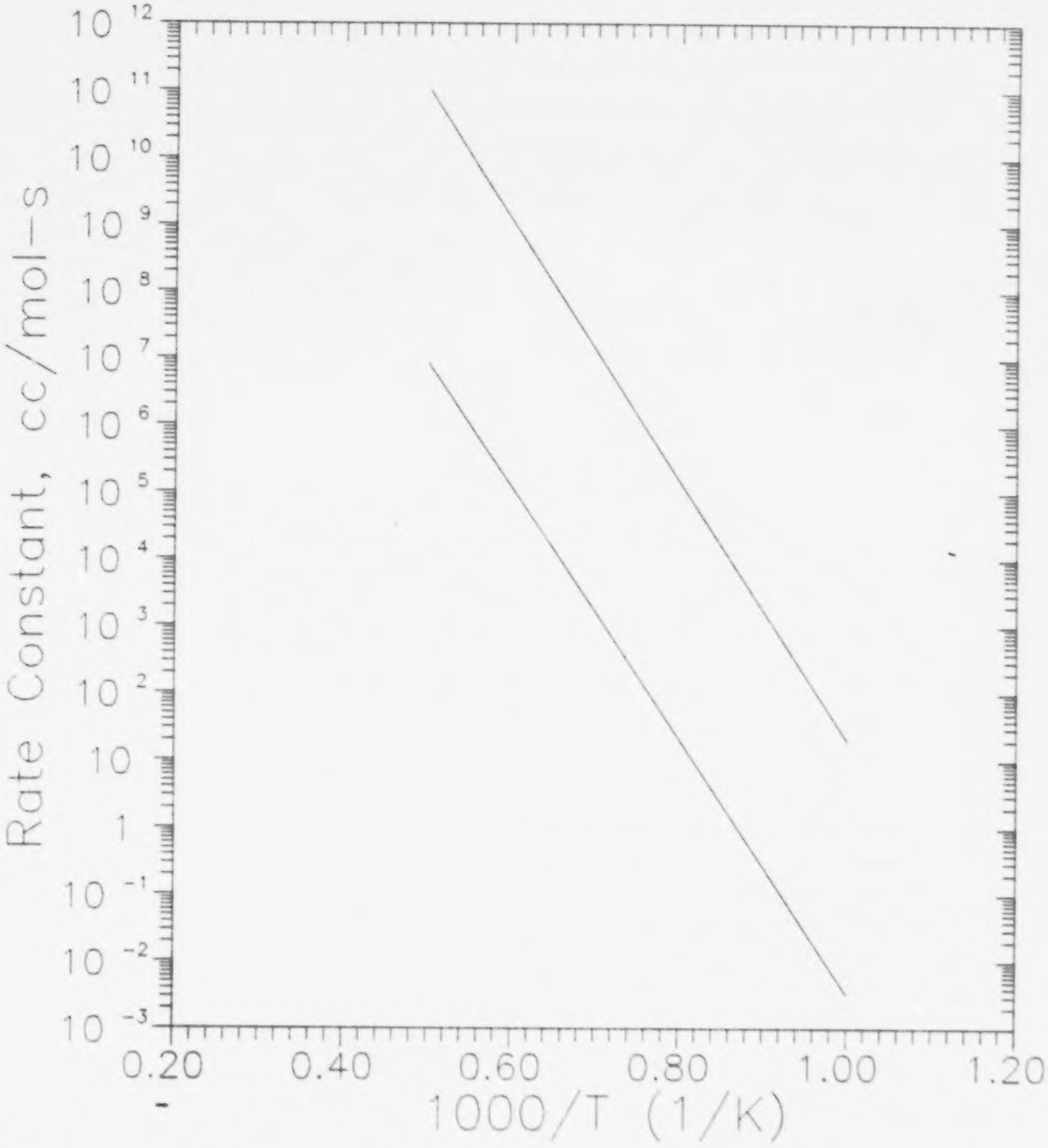
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH3 + N = NH + NH2**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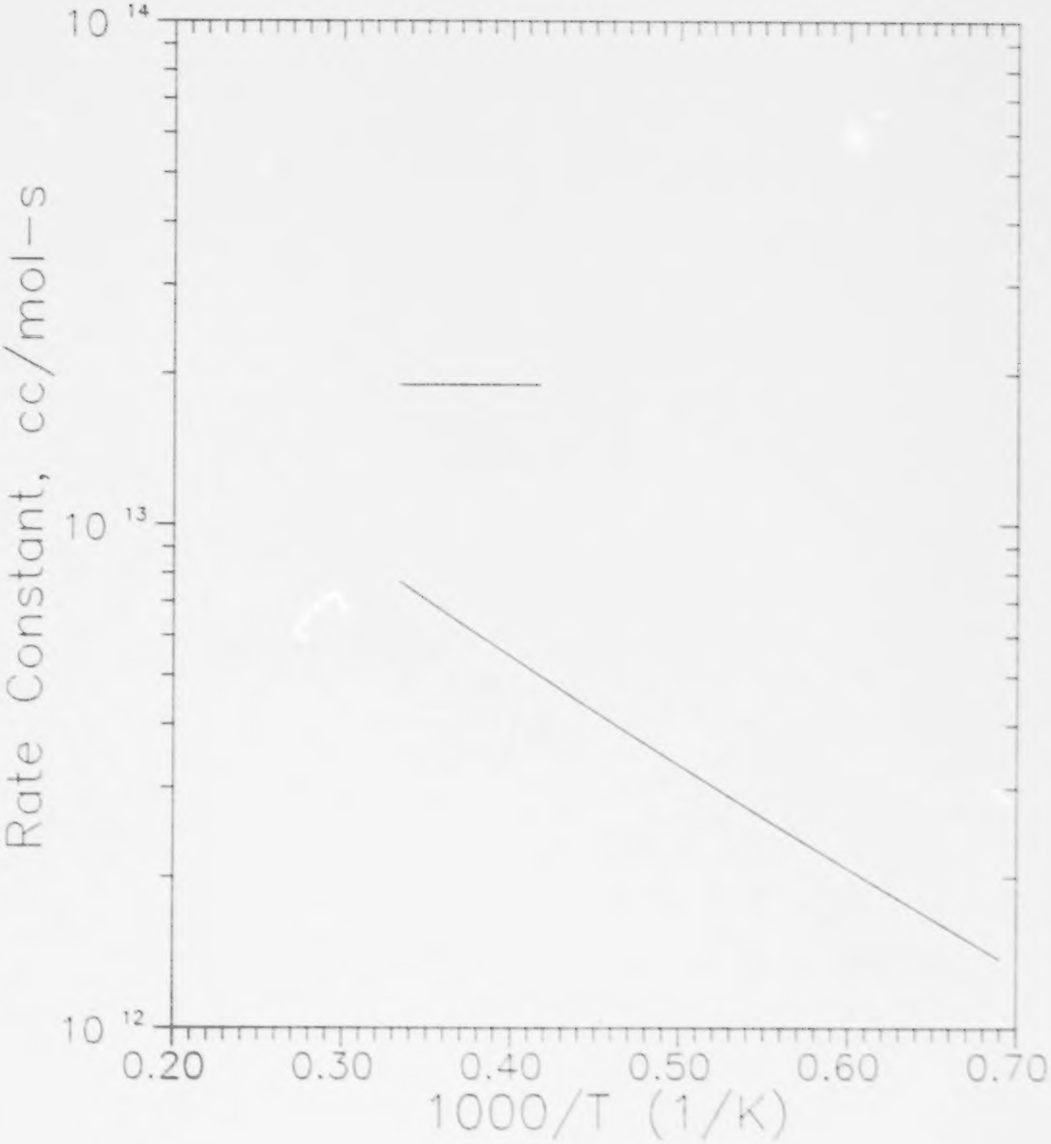
$10^{11}$
$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
$10^{5}$
$10^{4}$
$10^{3}$
$10^{2}$
10
1
$10^{-1}$
$10^{-2}$
$10^{-3}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH2 + M = NH + H + M**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10^13
10^12
Rate Constant, cc/mol-s
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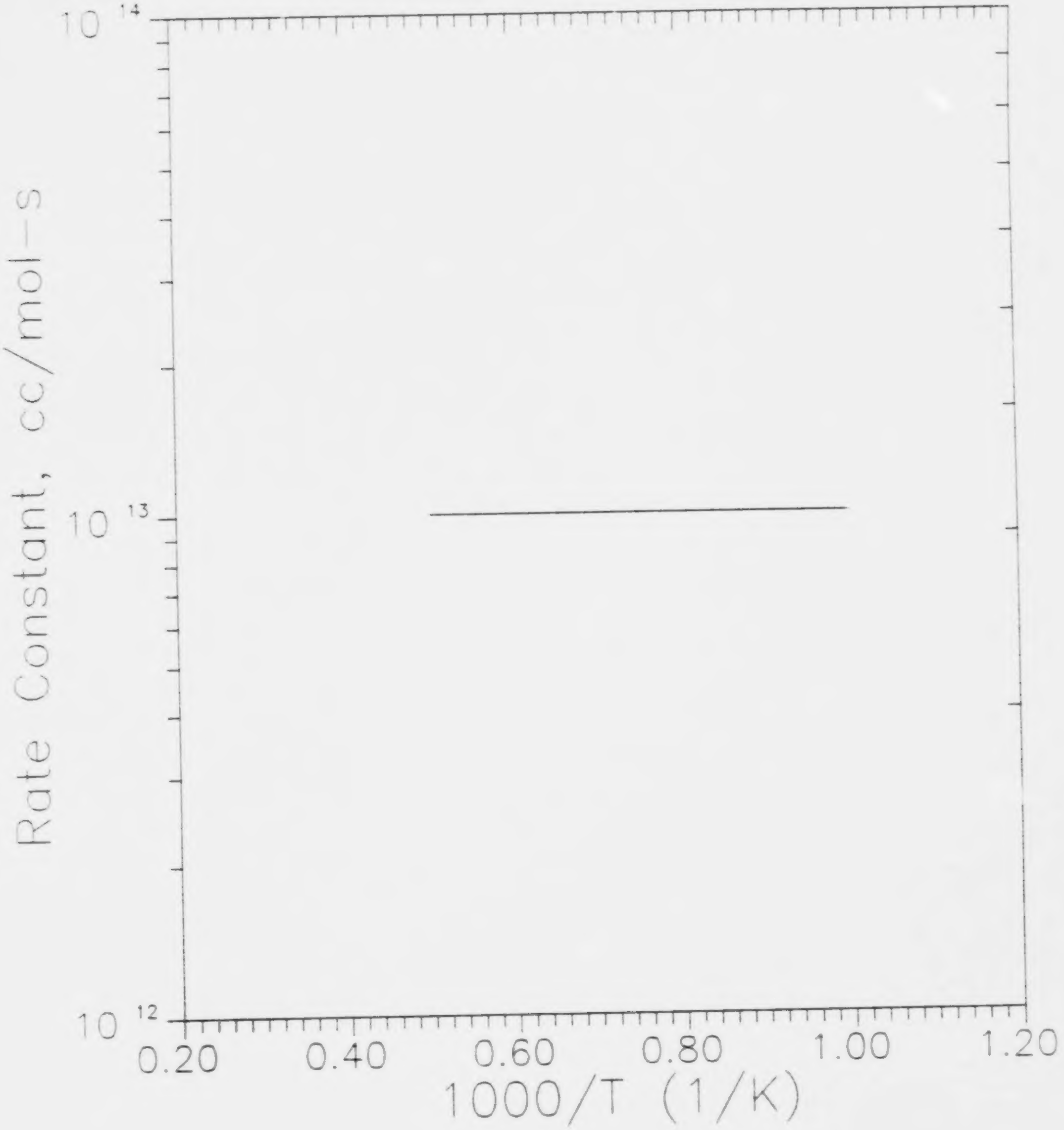
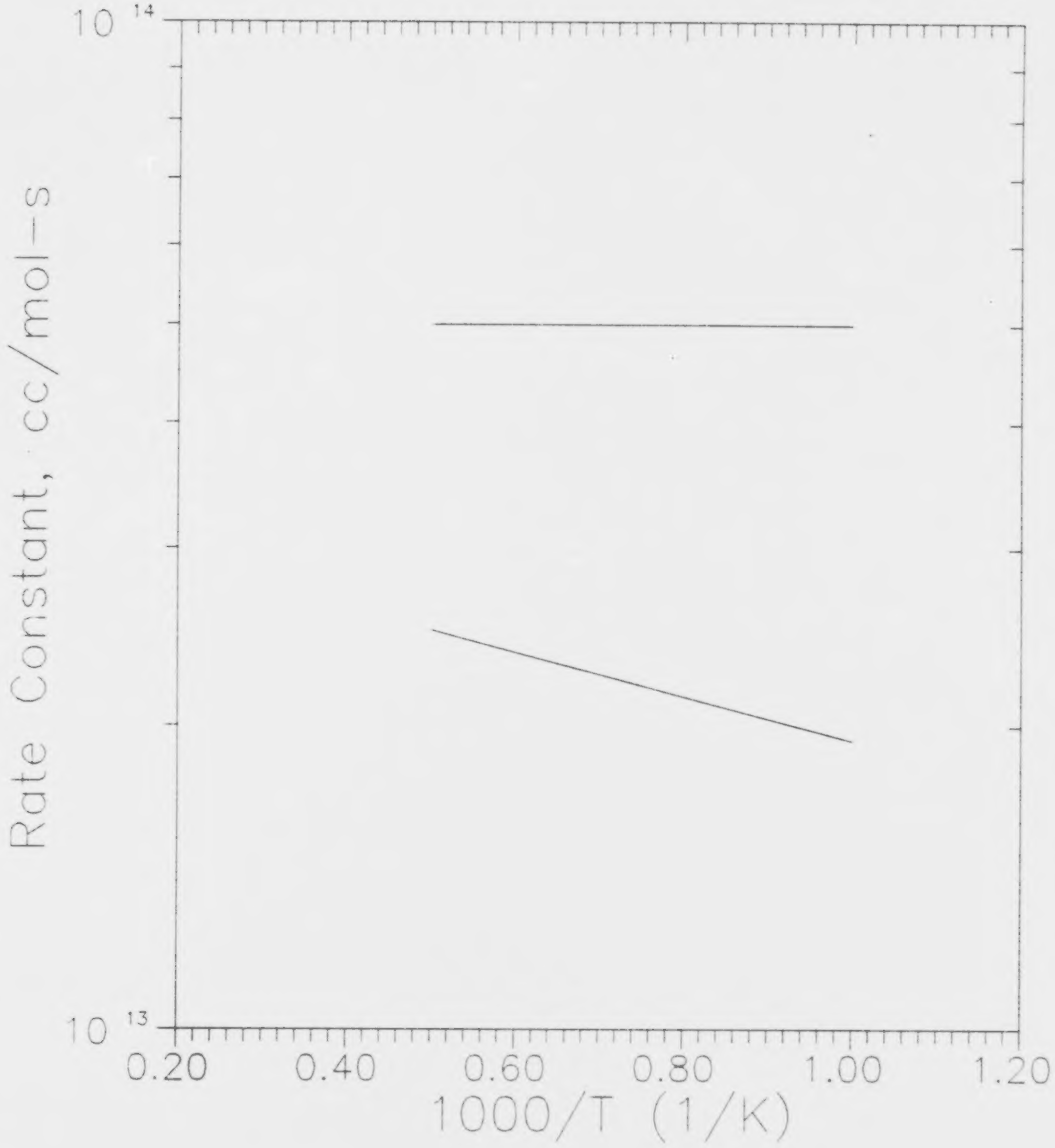
0.40
0.50
0.60
0.70
1000/T (1/K)

**NH2 + H = NH + H2**



**NH2 + HN2 = N2 + NH3**


10 $^{14}$
10 $^{13}$
Rate Constant, cc/mol-s
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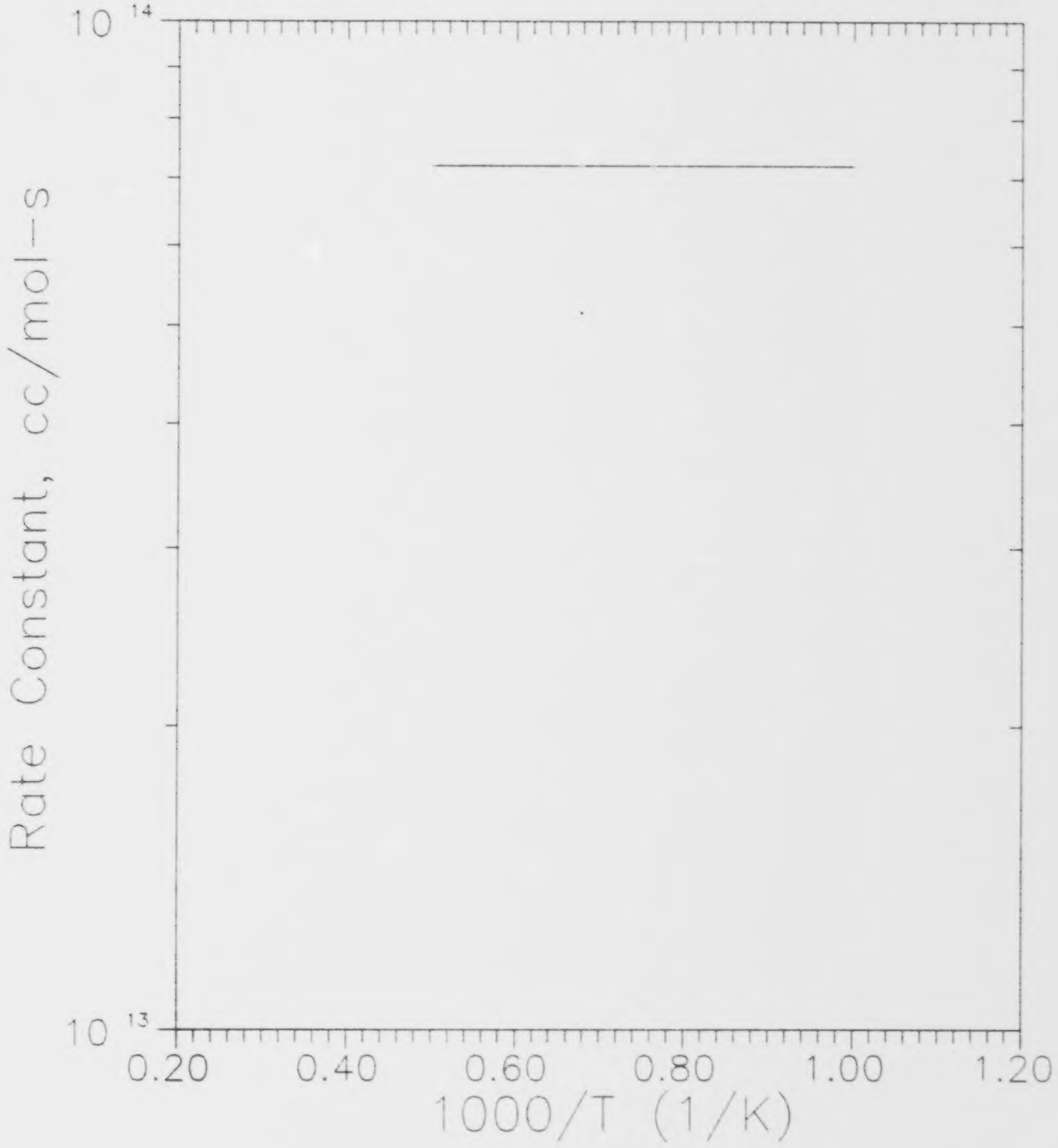
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH2 + NH = N2H2 + H**


10 ^14
10 ^13
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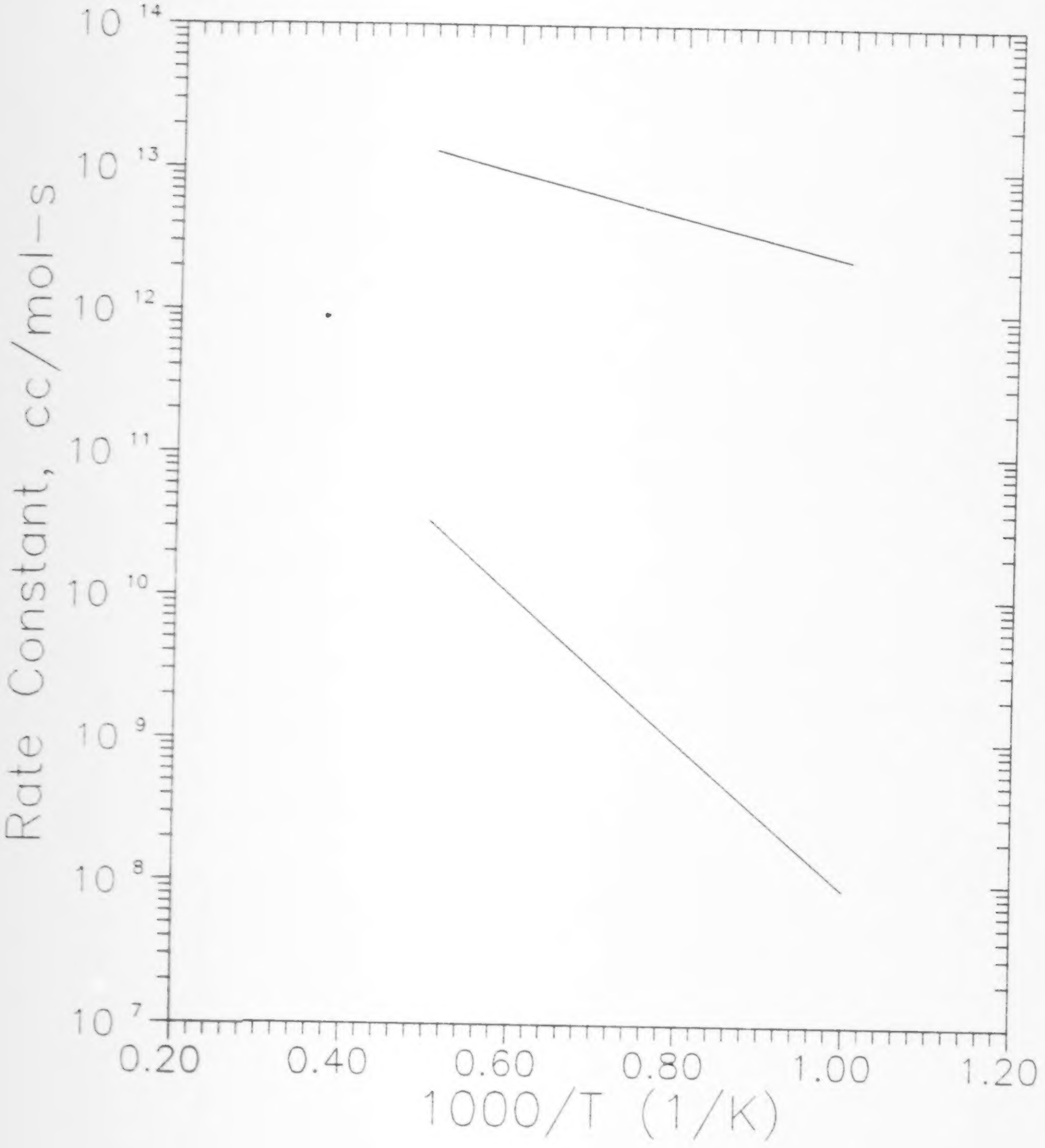
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)
Rate Constant, cc/mol-s

**NH2 + N = N2 + H + H**



Rate Constant, cc/mol-s
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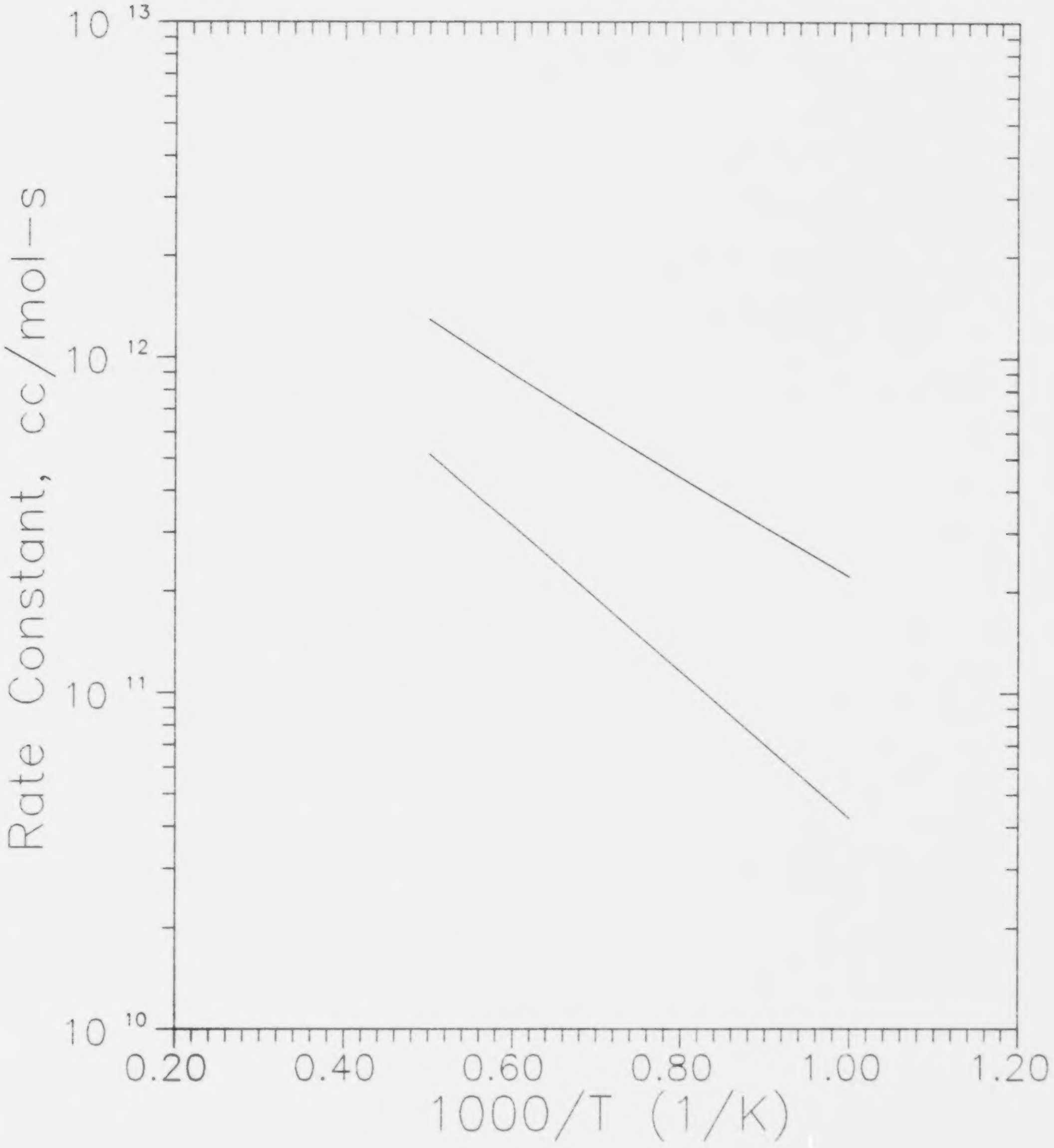
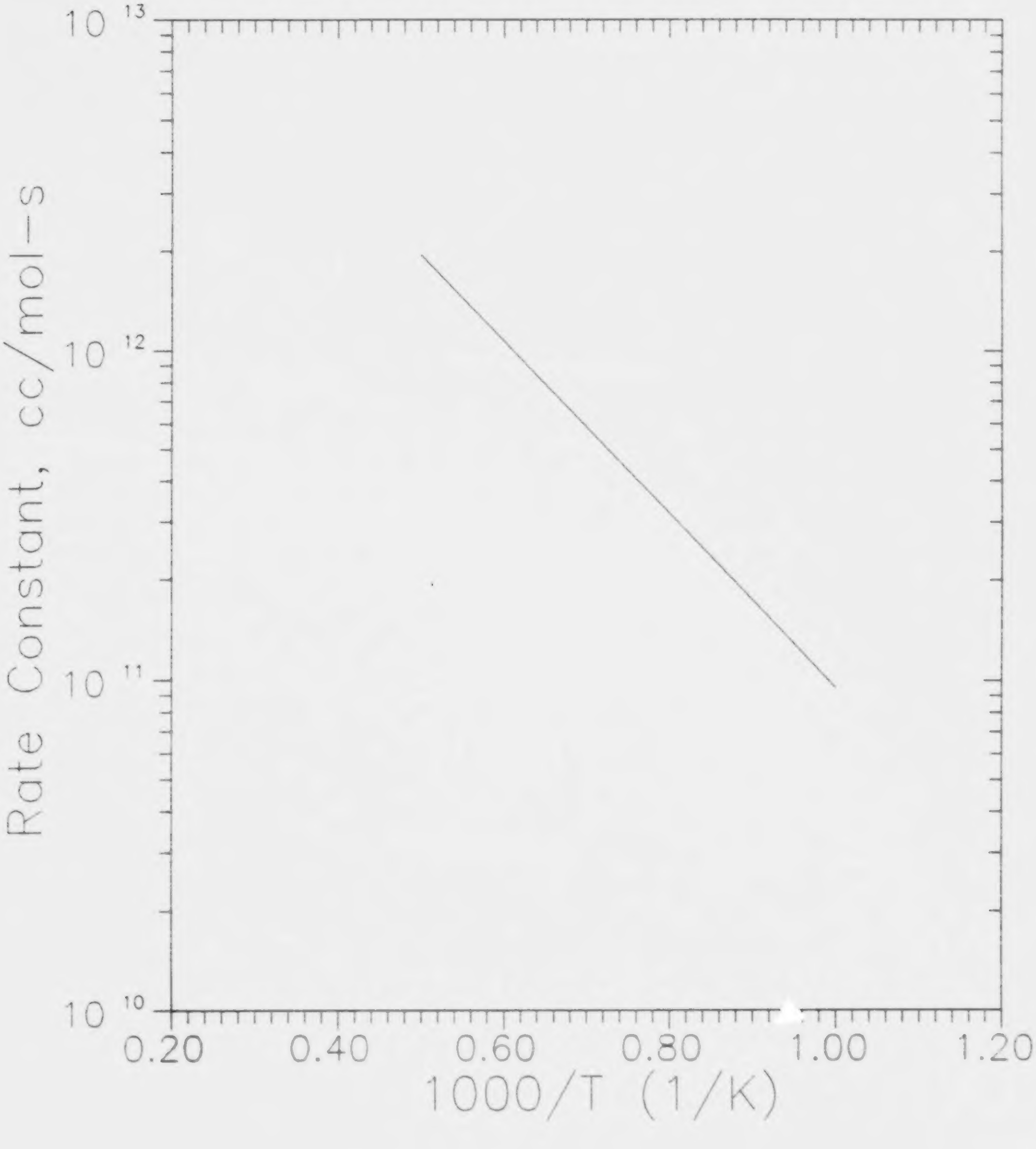
10 13
10 12
10 11
10 10
10 9
10 8
10 7
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

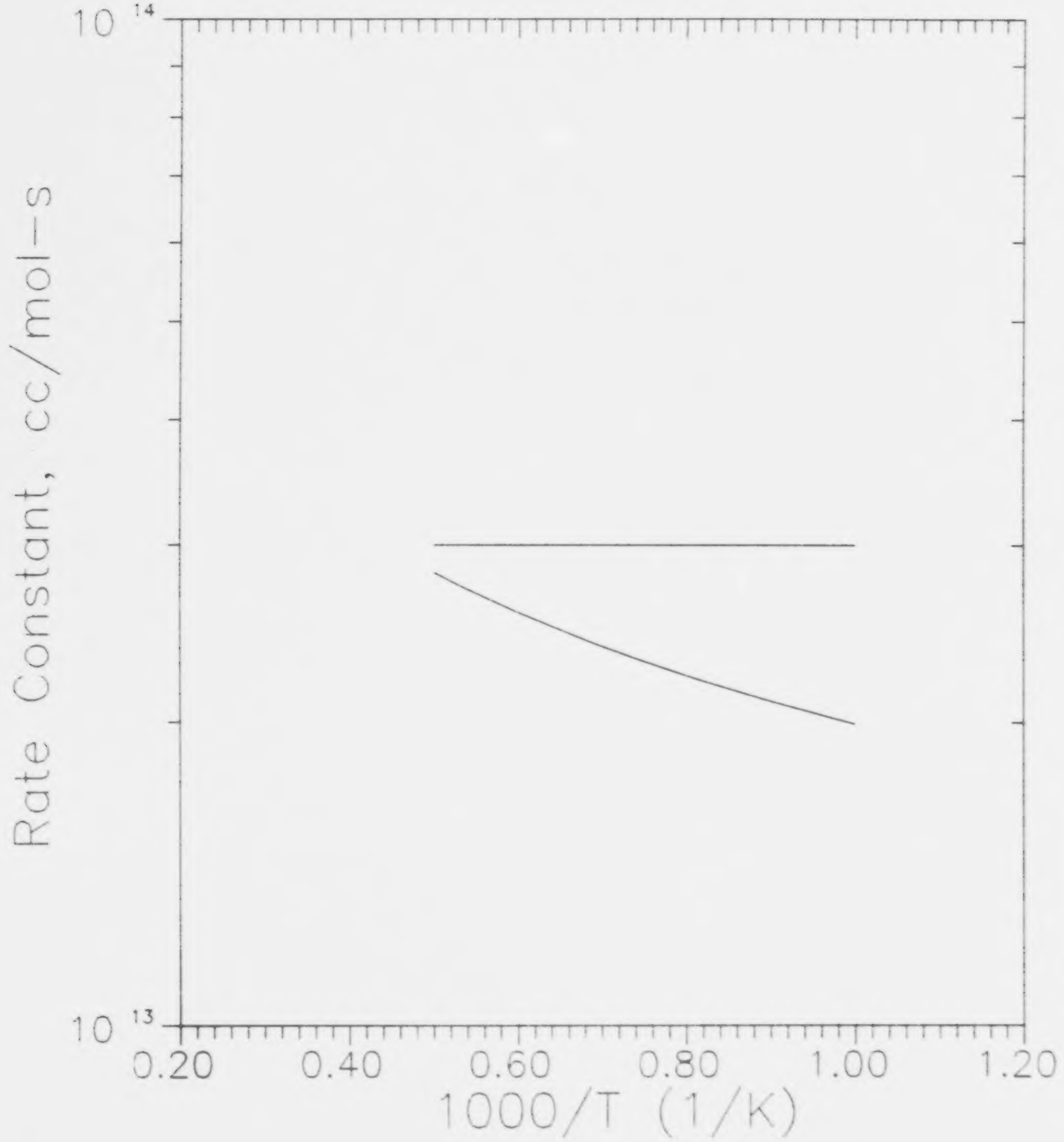
**NH2 + N = NH + NH**



**NH2 + NH2 = NH3 + NH**



**NH2 + NH2 = N2 + H2 + H2**


10^14
10^13
Rate Constant, cc/mol-s
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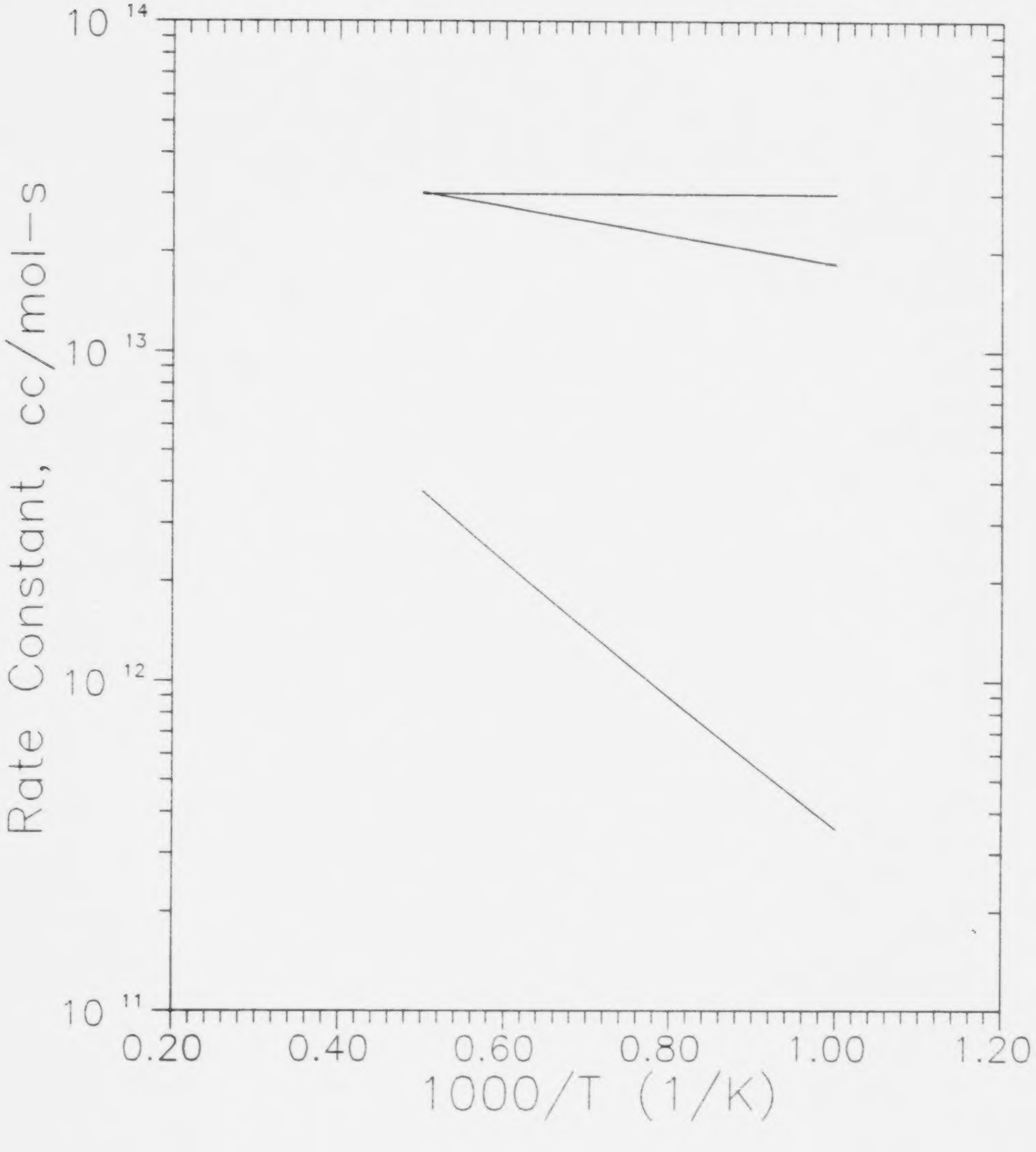
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH + N = N2 + H**



Rate Constant, cc/mol-s
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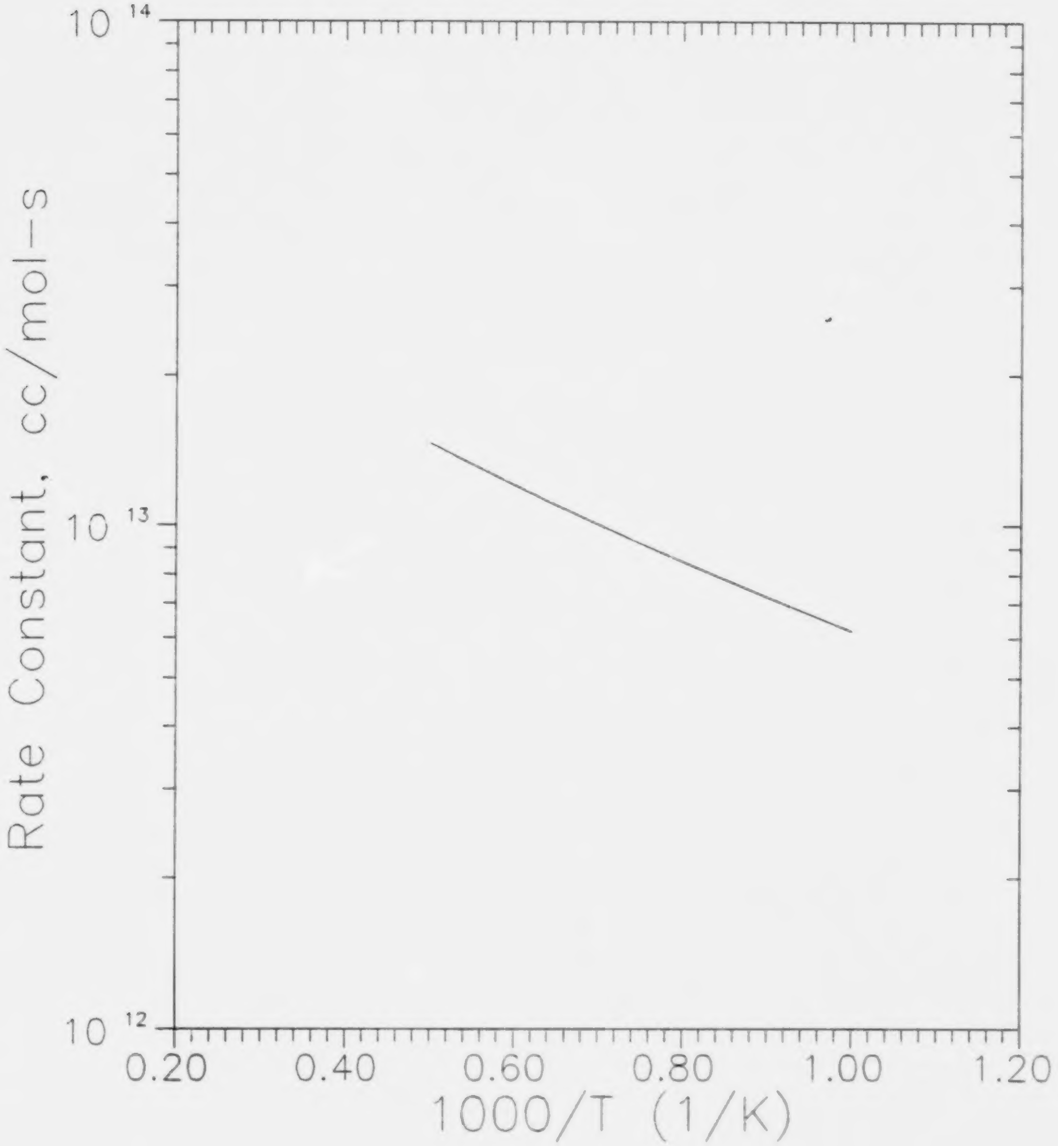
10 13
10 12
10 11
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH + H = N + H2**



$10^{14}$
$10^{13}$
$10^{12}$
Rate Constant, cc/mol-s
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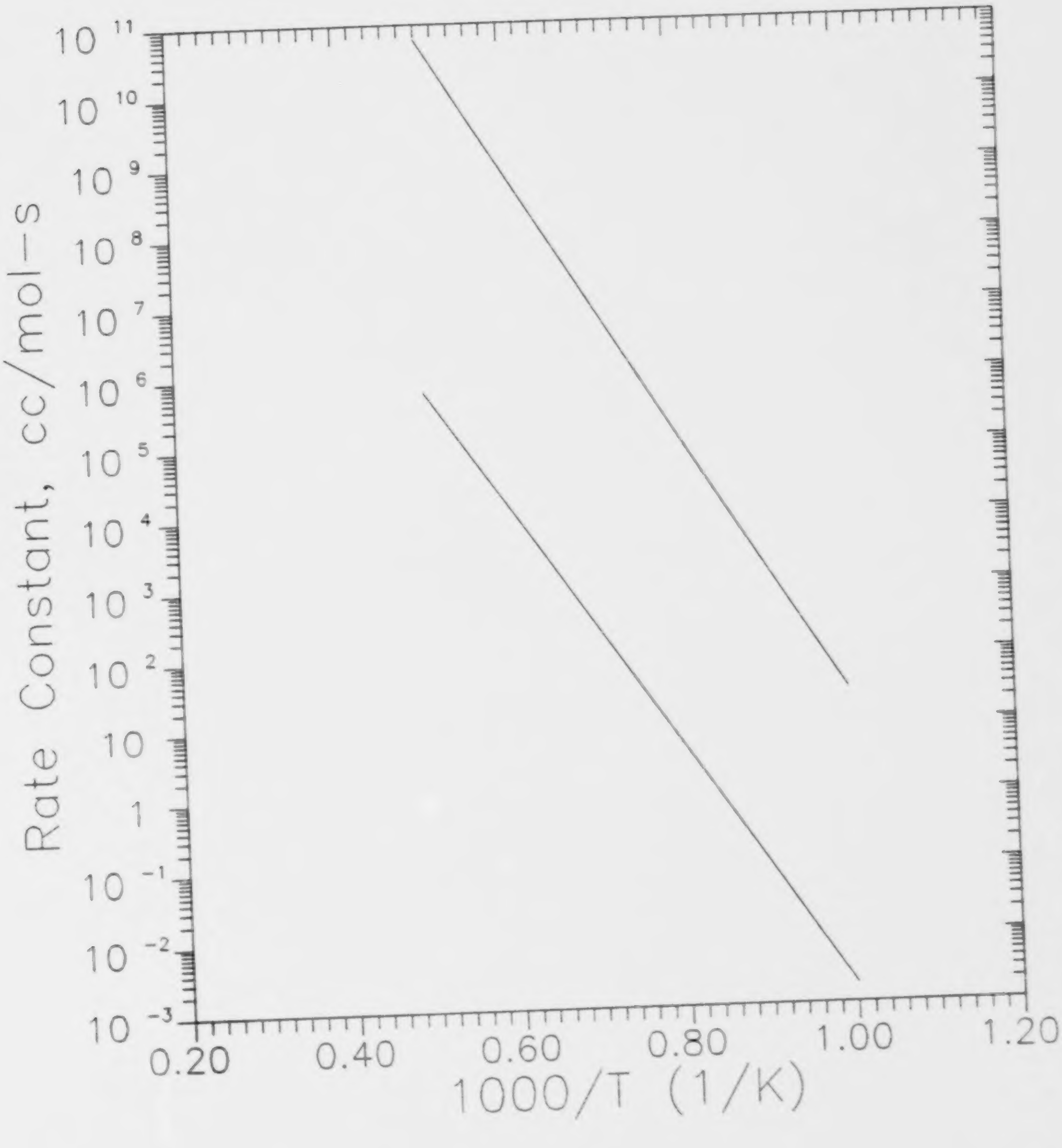
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH + NH = N2 + H2**


Rate Constant, cc/mol-s
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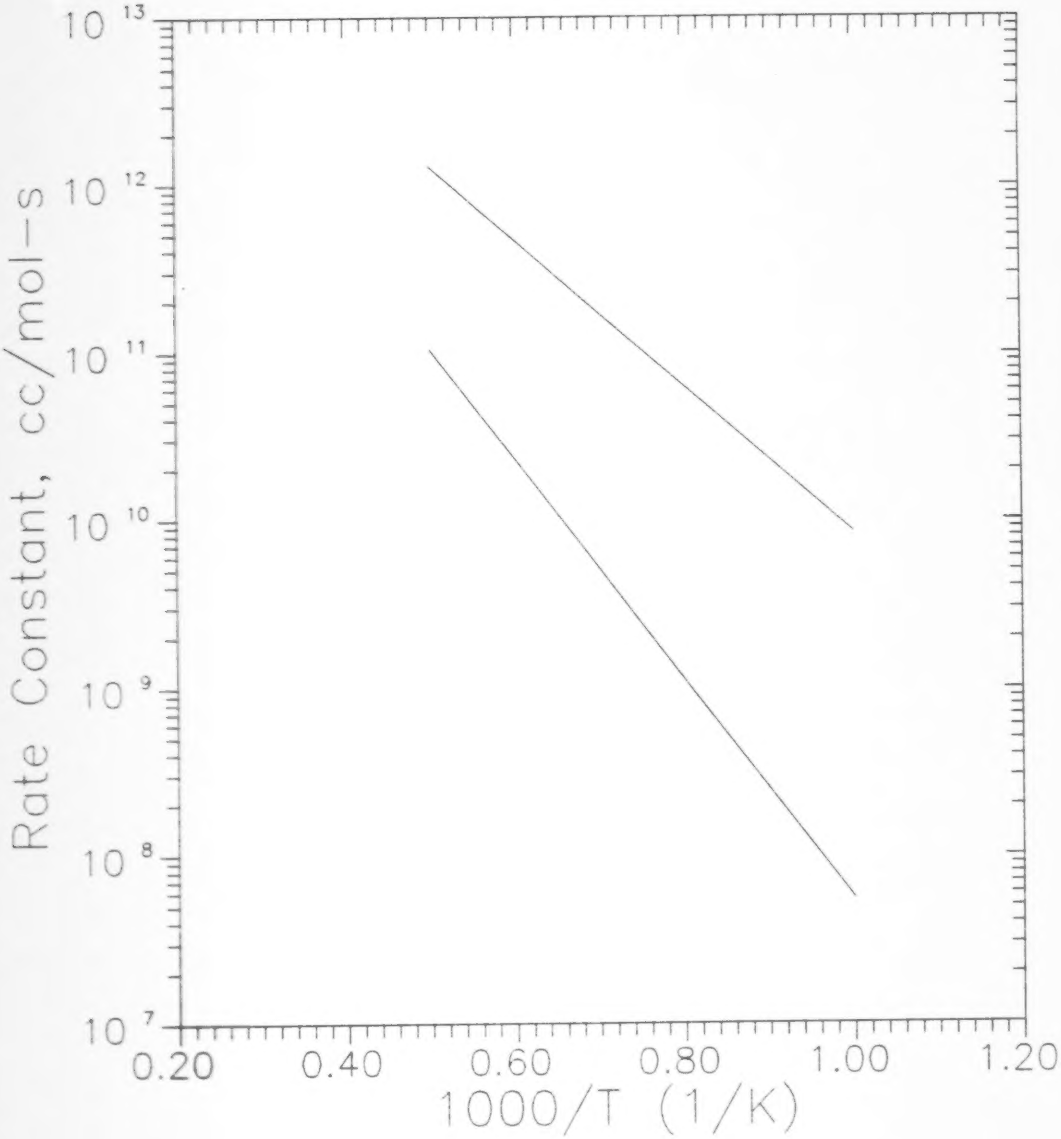
10^10
10^9
10^8
10^7
10^6
10^5
10^4
10^3
10^2
10
1
10^-1
10^-2
10^-3
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH + M = N + H + M**



Rate Constant, cc/mol-s
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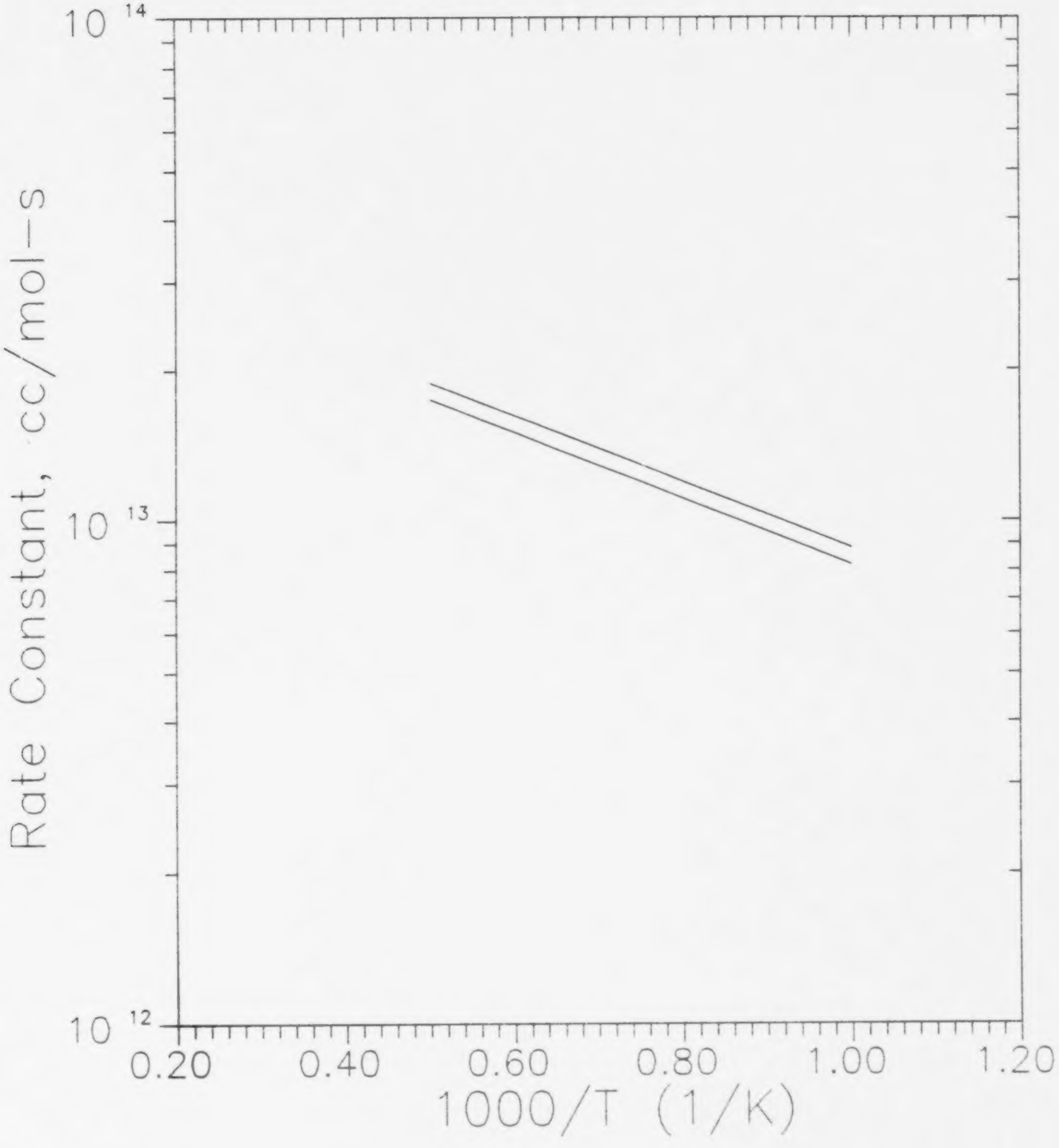
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HN2 + M = N2 + H + M**


10 14
10 13
10 12
Rate Constant, cc/mol-s
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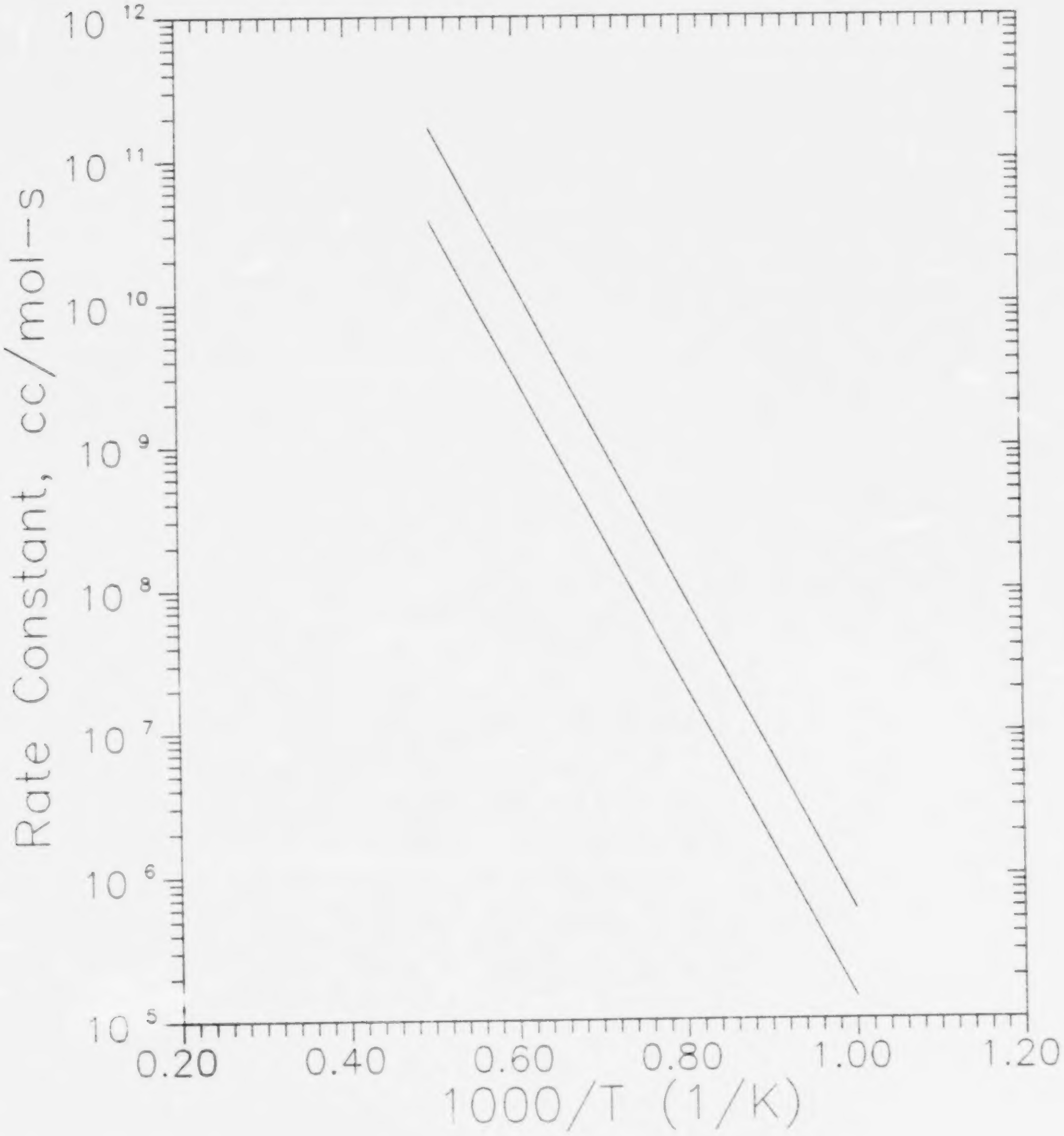
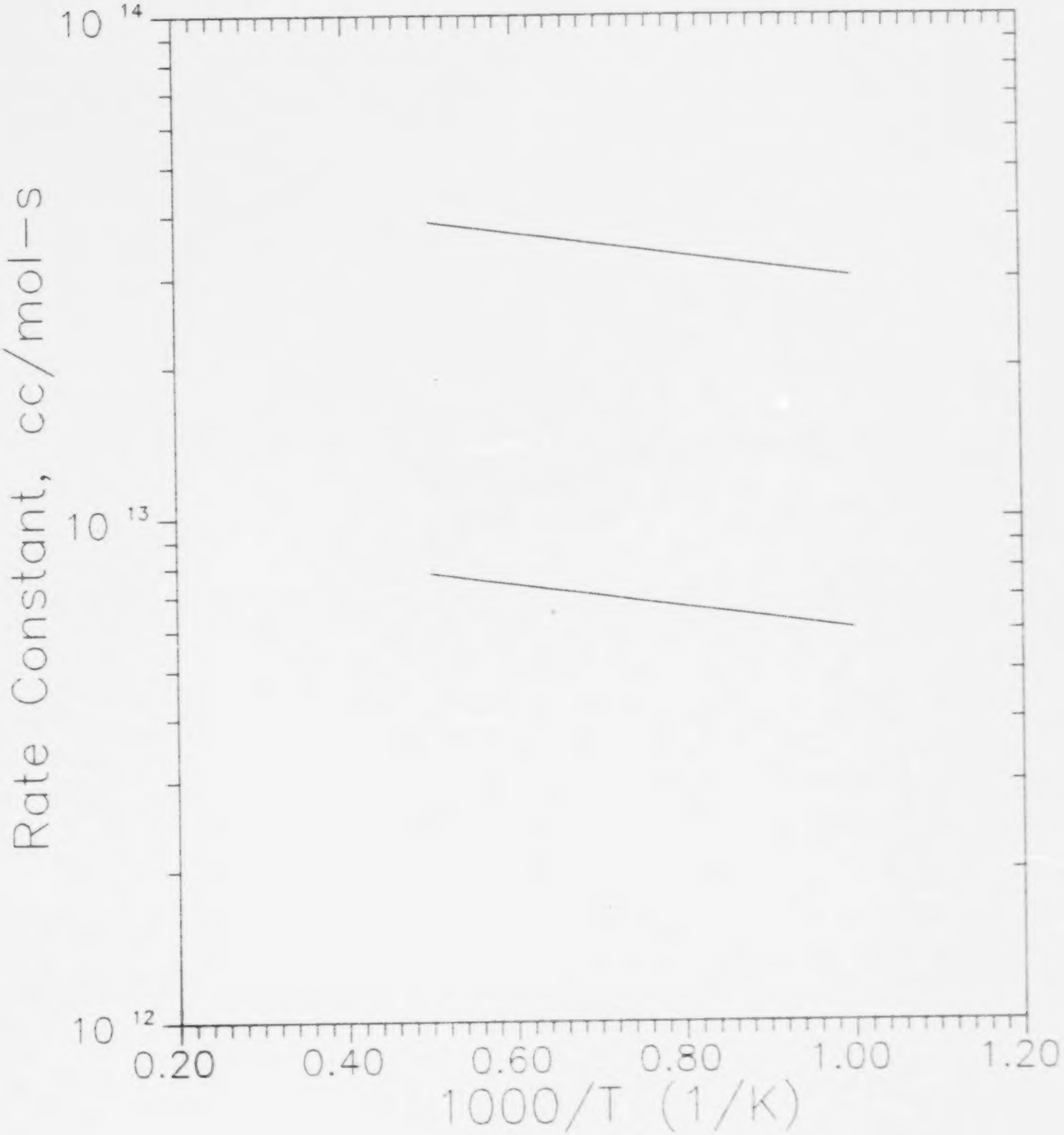
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HN2 + H = N2 + H2**


Rate Constant, cc/mol-s
10 ^12
10 ^11
10 ^10
10 ^9
10 ^8
10 ^7
10 ^6
10 ^5
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**N2H2 + M = HN2 + H + M**


10 14
10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**N2H2 + H = HN2 + H2**

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*----------------------------------------------------------------------------*
|  File: HNOMECH.DAT                                                         |
| Saved: 08-04-88 at 11:16:15 am                                    Page  1  |
*----------------------------------------------------------------------------*

 1NH3  + 1O            = 1NH2  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                  2.1E+13 0.000  9.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                    5.5E+09 0.750  5.030   300.0  1000.0
Lyon, 1987                             1.5E+12 0.000  6.040   300.0  1000.0
Hanson, Salimian in comb chem          2.0E+13 0.000  8.880  1000.0  2100.0

 1NH3  + 1HO           = 1NH2  + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                  8.1E+13 0.000  8.375  1750.0  2050.0
Glarborg, et al. 1986                  2.0E+06 2.040  0.560  1750.0  2050.0
Seeker, et al. 1985                    8.5E+09 0.750  1.100  1000.0  2000.0
Lyon, 1987                             3.3E+12 0.000  2.120   300.0  1075.0
Hanson, Salimian in comb chem          5.7E+13 0.000  8.050   900.0  2100.0

 1NH3  + 1HO2          = 1NH2  + 1H2O2
Forward Rate Parameters:
Seeker, et al. 1985                    1.0E+12 0.000 24.300  1000.0  2000.0
Hanson, Salimian in comb chem          2.5E+12 0.000 23.800  1000.0  2000.0

 1NH2  + 1O            = 1HNO  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                  7.9E+14-0.500  0.000   300.0  1000.0
Glarborg, et al. 1986                  6.6E+14-0.500  0.000   300.0  1000.0
Seeker, et al. 1985                    1.0E+11 0.500  0.000  1500.0  2000.0
Hanson, Salimian in comb chem          6.31E14-0.500  0.000   300.0  1000.0

 1NH2  + 1O            = 1NH   + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                  7.0E+12 0.000  0.000   300.0  1000.0
Glarborg, et al. 1986                  6.8E+12 0.000  0.000   300.0  1000.0
Seeker, et al. 1985                    1.0E+11 0.500  1.000  1000.0  2000.0
Lyon, 1987                             1.7E+13 0.000  1.000   300.0  1500.0
Hanson, Salimian in comb chem          1.3E+14-0.500  0.000   300.0  1000.0

 1NH2  + 1NO           = 1HN2  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                  8.8E+15-1.250  0.000  1000.0  2000.0
Glarborg, et al. 1986
Lyon, 1987                             6.1E+19-2.460  1.866  1000.0  2000.0

 1NH2  + 1NO           = 1N2   + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                  3.8E+15-1.250  0.000   300.0   500.0
Glarborg, et al. 1986
Seeker, et al. 1985                    2.4E+17-1.850  0.000   300.0   505.0
Lyon, 1987                             9.1E+19-2.460  1.866   300.0  1200.0
Hanson, Salimian in comb chem          6.3E+19-2.500  1.900   300.0  1200.0

 1NH2  + 1NO           = 1N2O  + 1H2
Forward Rate Parameters:
Seeker, et al. 1985                    5.0E+08 0.500  0.000  1500.0  2000.0
Hanson, Salimian in comb chem          5.0E+13 0.000 24.600  1560.0  2850.0
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*------------------------------------------------------------------------------*
! File: HNOMECH.DAT                                                             !
! Saved: 08-04-88 at 11:16:15 am                                      Page  2 !
*------------------------------------------------------------------------------*

 1NH2  + 1NO          = 1N2   + 1H    + 1HO
Forward Rate Parameters:
Seeker, et al. 1985                     1.4E+17-1.850  0.000   300.0   500.0
Hanson, Salimian in comb chem           6.3E+19-2.500  1.900   300.0  1200.0

 1NH2  + 1O2          = 1HNO  + 1HO
Forward Rate Parameters:
Seeker, et al. 1985                     5.0E+06 0.750  6.080  1000.0  2000.0
Lyon, 1987                              5.1E+13 0.000 30.000  1000.0  2001.0
Hanson, Salimian in comb chem           1.78E12 0.000 15.000  1550.0  1800.0

 1NH2  + 1HO          = 1NH   + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                   4.5E+12 0.000  2.120  1000.0  2000.0
Glarborg, et al. 1986                   4.5E+12 0.000  2.200  1000.0  2000.0
Seeker, et al. 1985                     6.3E+11 0.500  0.000  1000.0  2000.0
Lyon, 1987                              5.5E+10 0.680  1.290  1000.0  2000.0
Hanson, Salimian in comb chem           5.0E+11 0.500  2.000  1000.0  2000.0

 1NH2  + 1HNO         = 1NH3  + 1NO
Forward Rate Parameters:
Seeker, et al. 1985                     5.0E+11 0.500  2.740  1000.0  2000.0
Lyon, 1987                              1.8E+14 0.000  1.000  1000.0  2000.0
Hanson, Salimian in comb chem           5.0E+11 0.500  0.990  1000.0  2000.0

 1NH2  + 1HO2         = 1NH   + 1H2O2
Forward Rate Parameters:
Seeker, et al. 1985                     1.0E+14 0.000  1.200  1000.0  2000.0
Hanson, Salimian in comb chem           1.0E+13 0.000  2.000  1000.0  2000.0

 1NH2  + 1HO2         = 1NH3  + 1O2
Forward Rate Parameters:
Seeker, et al. 1985                     2.0E+10 0.500  2.590  1000.0  2000.0
Hanson, Salimian in comb chem           1.0E+13 0.000  2.000  1000.0  2000.0

 1NH   + 1O2          = 1HNO  + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                   1.0E+13 0.000 12.000   300.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                     5.0E+11 0.500  4.370  1000.0  2000.0
Lyon, 1987                              3.0E+13 0.000  3.400  1000.0  2000.0
Hanson, Salimian in comb chem           1.0E+13 0.000 11.900  1000.0  2000.0

 1NH   + 1O2          = 1NO   + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                   1.4E+11 0.000  2.000   300.0  1000.0
Glarborg, et al. 1986

 1NH   + 1NO          = 1N2O  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   4.3E+14-0.500  0.000   300.0  1000.0
Glarborg, et al. 1986
Seeker, et al. 1985                     5.4E+16-1.400  0.000  1000.0  2000.0
Hanson, Salimian in comb chem           1.1E+12 0.000  0.460  1600.0  3000.0
```

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*---------------------------------------------------------------------------*
| File: HNOMECH.DAT                                                          |
| Saved: 08-04-88 at 11:16:15 am                                   Page  3   |
*---------------------------------------------------------------------------*

 1NH   + 1N2O          = 1N2   + 1HNO
Forward Rate Parameters:
Seeker, et al. 1985                      2.0E+10 1.000 12.000  1000.0  2000.0
Hanson, Salimian in comb chem            2.0E+12 0.000  6.000  1000.0  2000.0

 1NH   + 1HO           = 1HNO  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                    2.0E+13 0.000  0.000   300.0  1000.0
Glarborg, et al. 1986
Seeker, et al. 1985                      5.0E+11 0.500  5.620  1000.0  2000.0
Hanson, Salimian in comb chem            1.0E+12 0.500  2.000  1000.0  2000.0

 1NH   + 1HO           = 1N    + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                    5.0E+11 0.500  2.000  1000.0  2000.0
Glarborg, et al. 1986
Hanson, Salimian in comb chem
Seeker, et al. 1985                      5.0E+11 0.500  4.450  1000.0  2000.0

 1NH   + 1HO2          = 1HNO  + 1HO
Forward Rate Parameters:
Seeker, et al. 1985                      6.3E+11 0.500  0.000  1000.0  2000.0
Hanson, Salimian in comb chem            1.0E+13 0.000  2.000  1000.0  2000.0

 1NH   + 1O            = 1NO   + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                    2.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                      6.3E+11 0.500  0.000  1000.0  2000.0
Hanson, Salimian in comb chem

 1NH   + 1O            = 1N    + 1HO
Forward Rate Parameters:
Seeker, et al. 1985                      6.3E+11 0.500  8.000  1000.0  2000.0
Hanson, Salimian in comb chem

 1N    + 1HO           = 1NO   + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                    3.8E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                      6.3E+11 0.500  0.000  1000.0  2000.0
Reverse Rate Parameters:
Hanson, Salimian in comb chem            2.6E+14 0.000 47.200  1750.0  3000.0

 1HN2  + 1HO           = 1N2   + 1H2O
Forward Rate Parameters:
Lyon, 1987                               3.0E+13 0.000  0.000   300.0  1500.0
Hanson, Salimian in comb chem

 1HN2  + 1NO           = 1N2   + 1HNO
Forward Rate Parameters:
Glarborg, et al. 1985                    5.0E+13 0.000  0.000   300.0  1500.0
Glarborg, et al. 1986
Lyon, 1987                               9.1E+11 0.000  0.000   914.0  1388.0
```
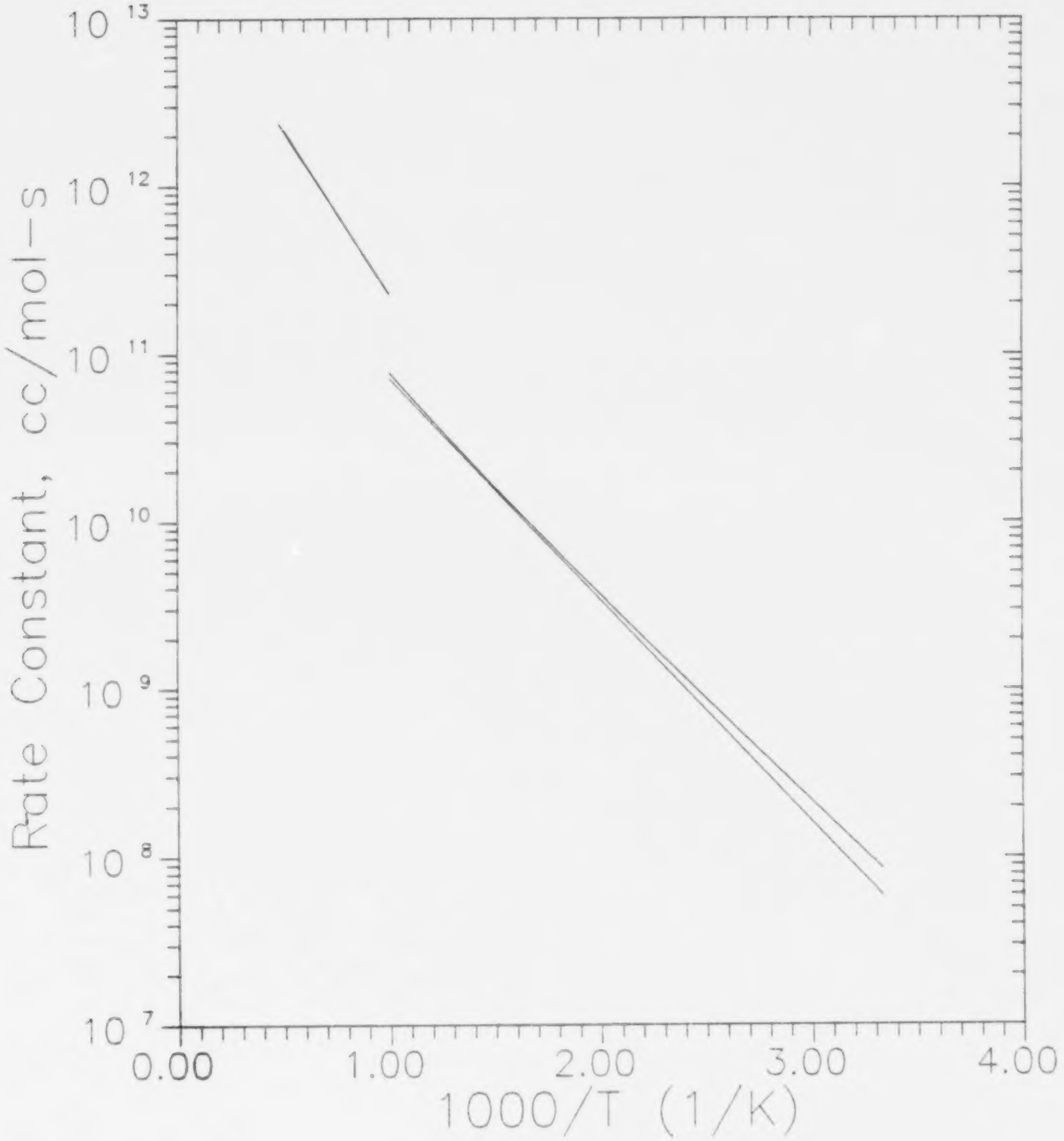
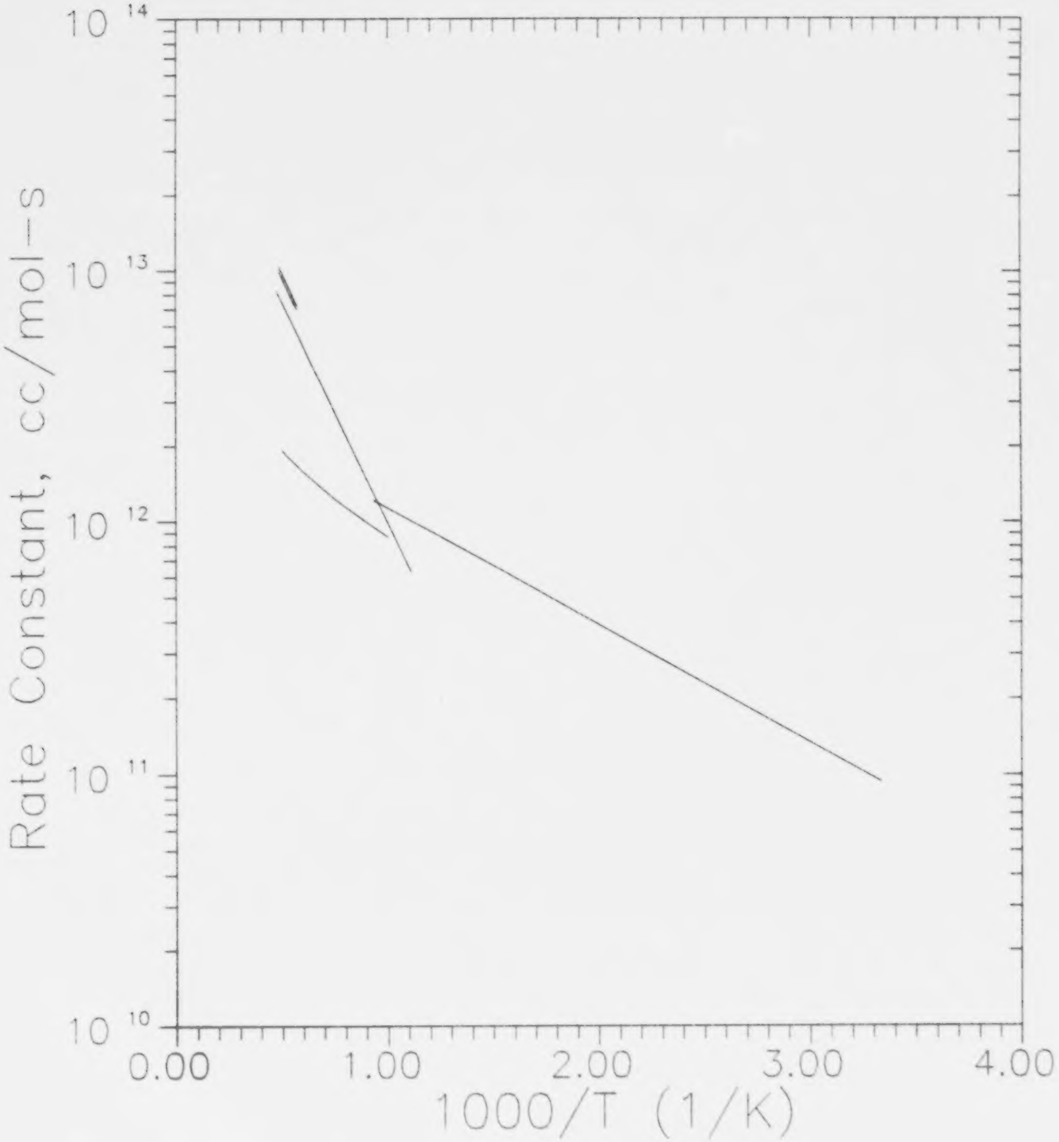
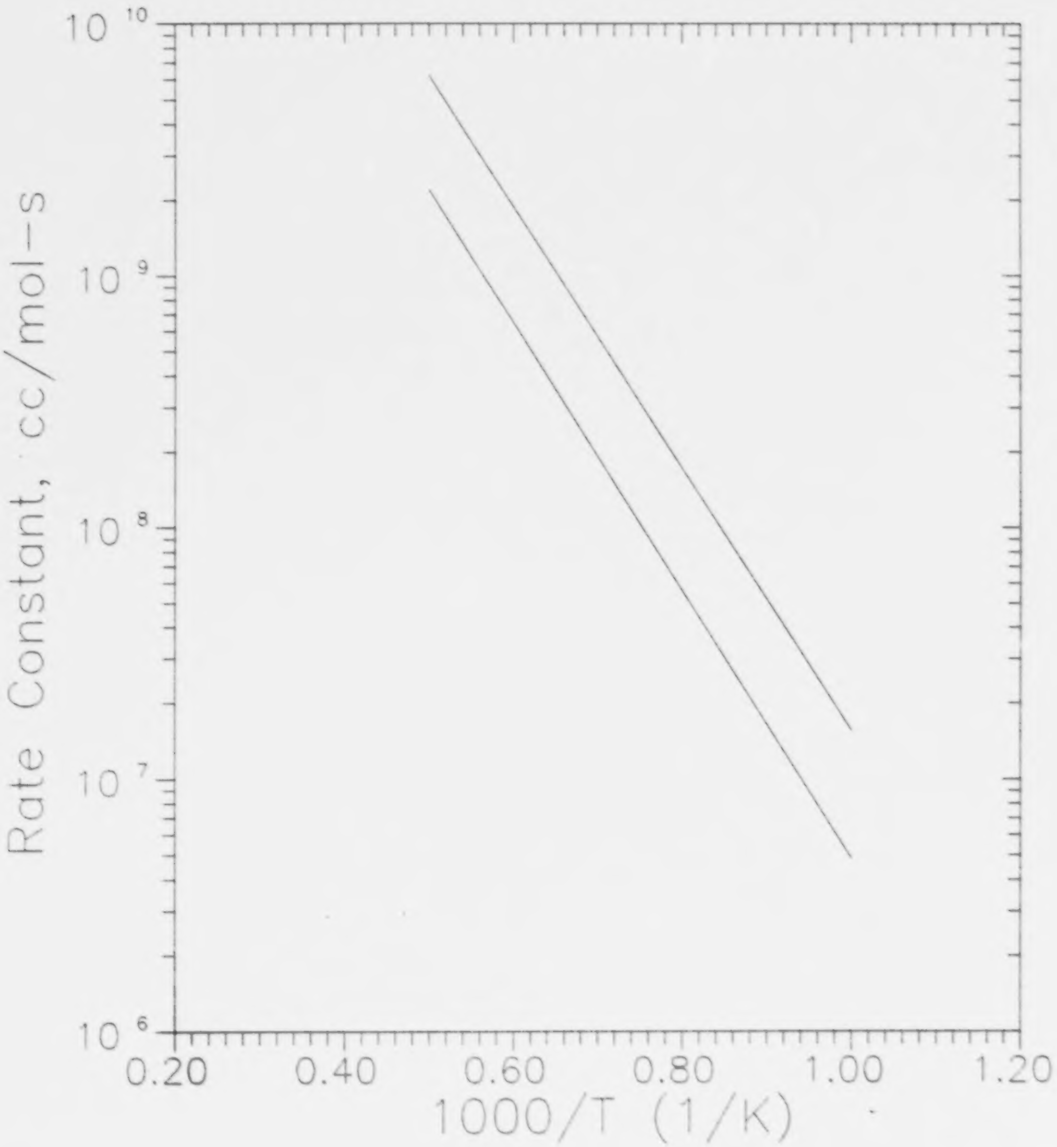

```
 1NO    + 1HO2            = 1NO2  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                   2.1E+12 0.000 -0.480   300.0  2000.0
Glarborg, et al. 1986
Hanson, Salimian in comb chem
Lyon, 1987                              3.4E+12 0.000 -0.260  1000.0  2000.0
Seeker, et al. 1985                     3.0E+11 0.500  0.000  1000.0  2000.0

 1NO    + 1H     + 1M     = 1HNO  + 1M
Forward Rate Parameters:
Seeker, et al. 1985                     2.2E+17 0.500  0.000  1000.0  2000.0

 1NO2   + 1H              = 1NO   + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                   3.5E+14 0.000  1.500  1000.0  2000.0
Glarborg, et al. 1986
Lyon, 1987
Hanson, Salimian in comb chem
Seeker, et al. 1985                     2.9E+14 0.000  0.800  1000.0  2000.0

 1N2O   + 1H              = 1N2   + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                   7.6E+13 0.000 15.200   700.0  2500.0
Glarborg, et al. 1986
Seeker, et al. 1985
Hanson, Salimian in comb chem

 1HNO   + 1O              = 1HO   + 1NO
Forward Rate Parameters:
Seeker, et al. 1985                     5.0E+11 0.500  2.740  1000.0  2000.0

 1HNO   + 1M              = 1H    + 1NO   + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                   1.5E+16 0.000 48.680  1000.0  2000.0
Glarborg, et al. 1986
Lyon, 1987                              1.9E+16 0.000 48.680  1000.0  2000.0
Hanson, Salimian in comb chem           1.8E+16 0.000 48.700  1000.0  2000.0

 1HNO   + 1HO             = 1NO   + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                   3.6E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Lyon, 1987
Seeker, et al. 1985                     1.0E+12 0.500  2.740  1000.0  2000.0
Hanson, Salimian in comb chem           1.3E+12 0.500  2.000  1000.0  2000.0

 1HNO   + 1H              = 1H2   + 1NO
Forward Rate Parameters:
Glarborg, et al. 1985                   5.0E+12 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                     1.0E+13 0.000  2.500  1000.0  2000.0
Hanson, Salimian in comb chem           1.3E+13 0.000  4.000  1000.0  2000.0
```


10 13
10 12
10 11
10 10
10 9
10 8
10 7
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

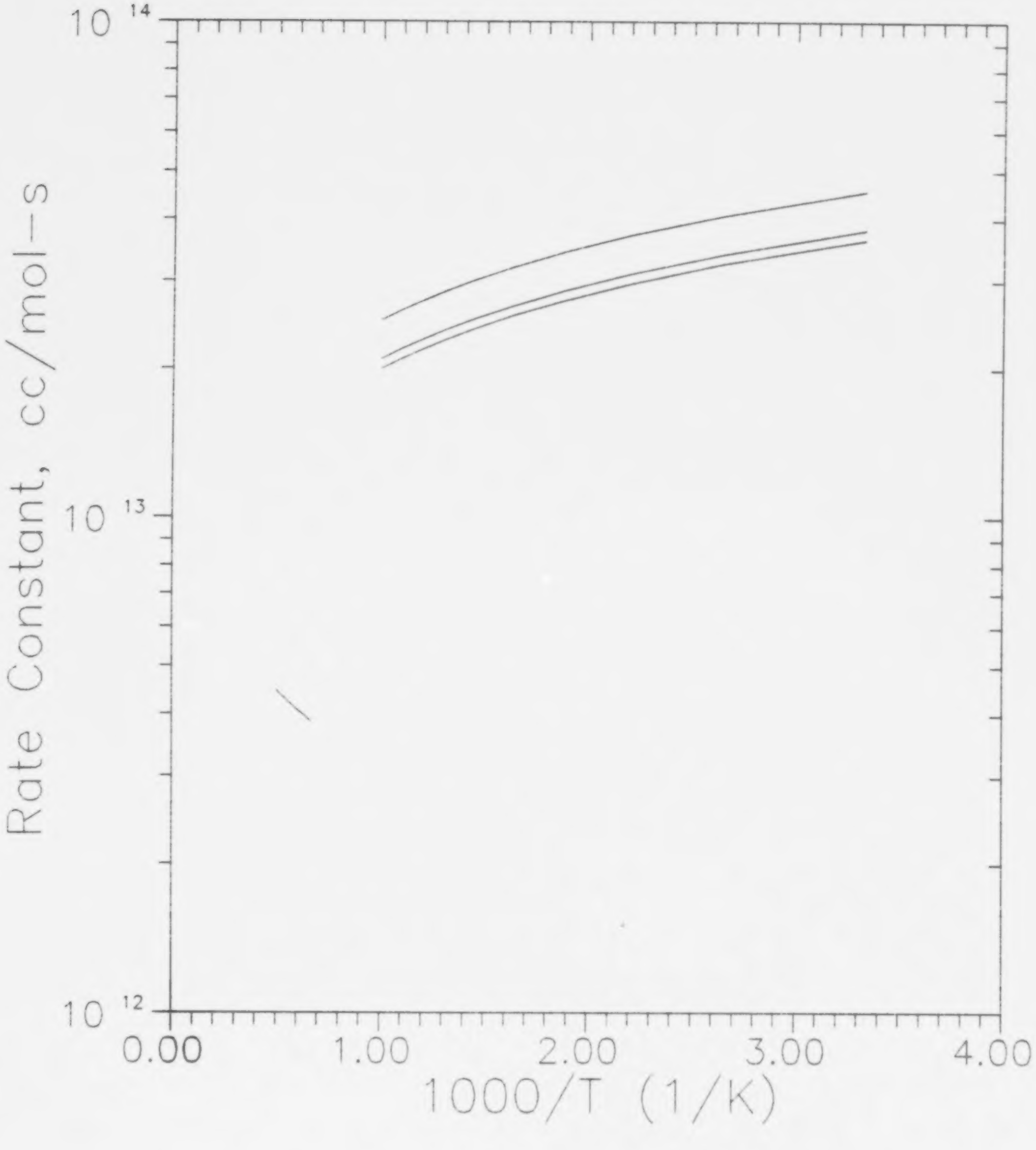
**NH3 + O = NH2 + HO**



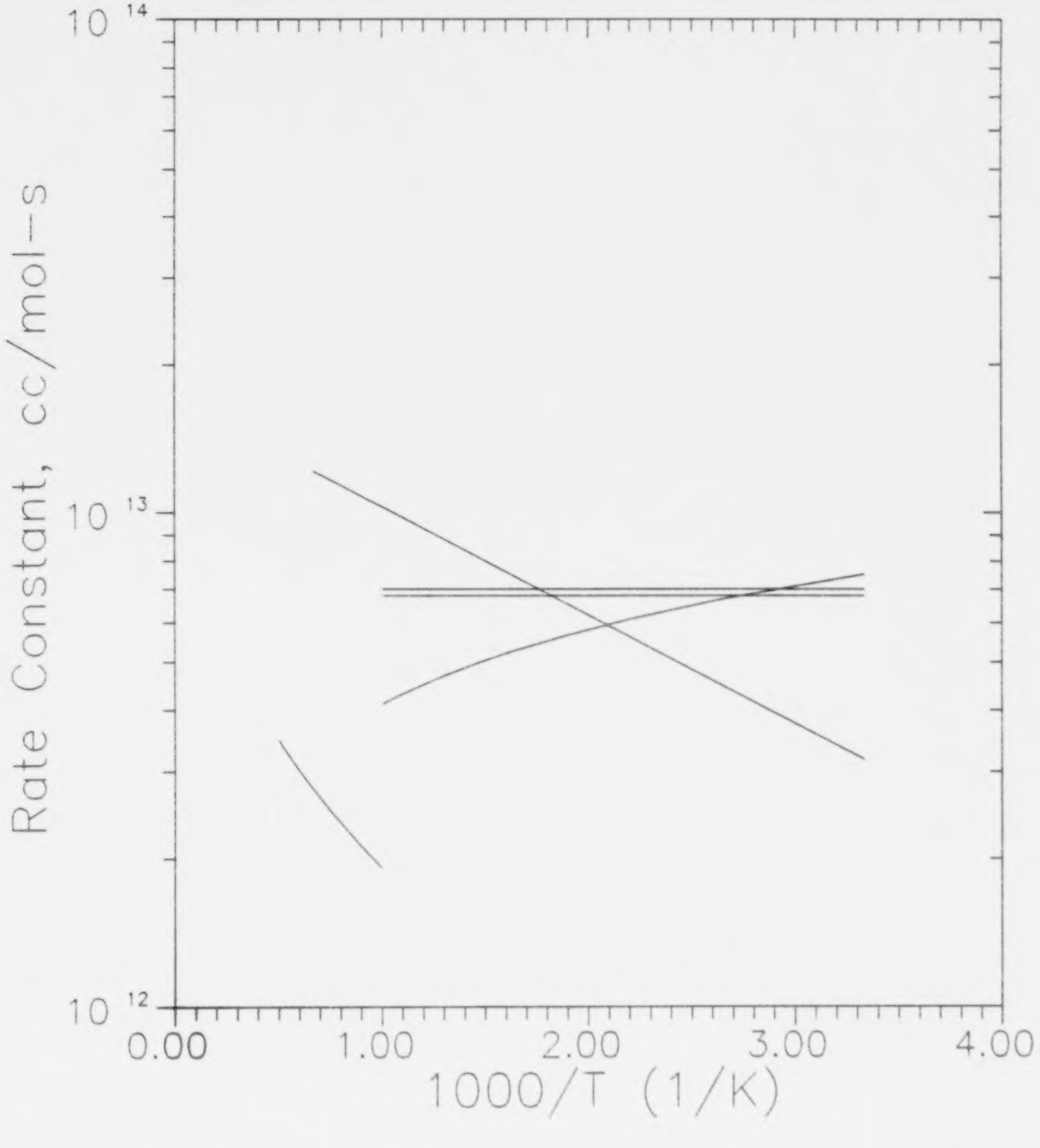
**NH3 + HO = NH2 + H2O**



**NH3 + HO2 = NH2 + H2O2**

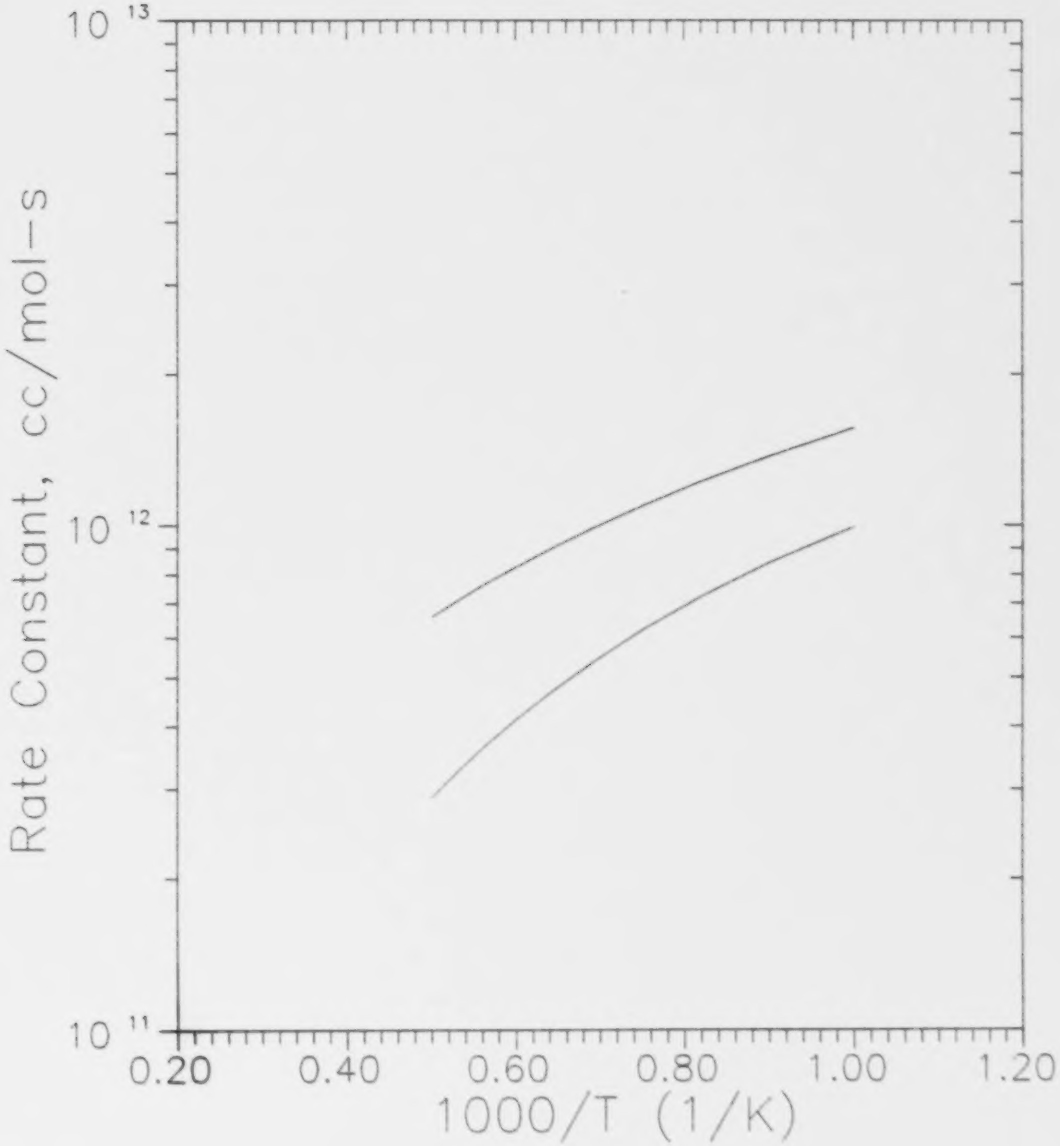

10 14
10 13
10 12
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**NH2 + O = HNO + H**



10 ^14
10 ^13
10 ^12
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**NH2 + O = NH + HO**



10 ^13
10 ^12
10 ^11
Rate Constant, cc/mol-s
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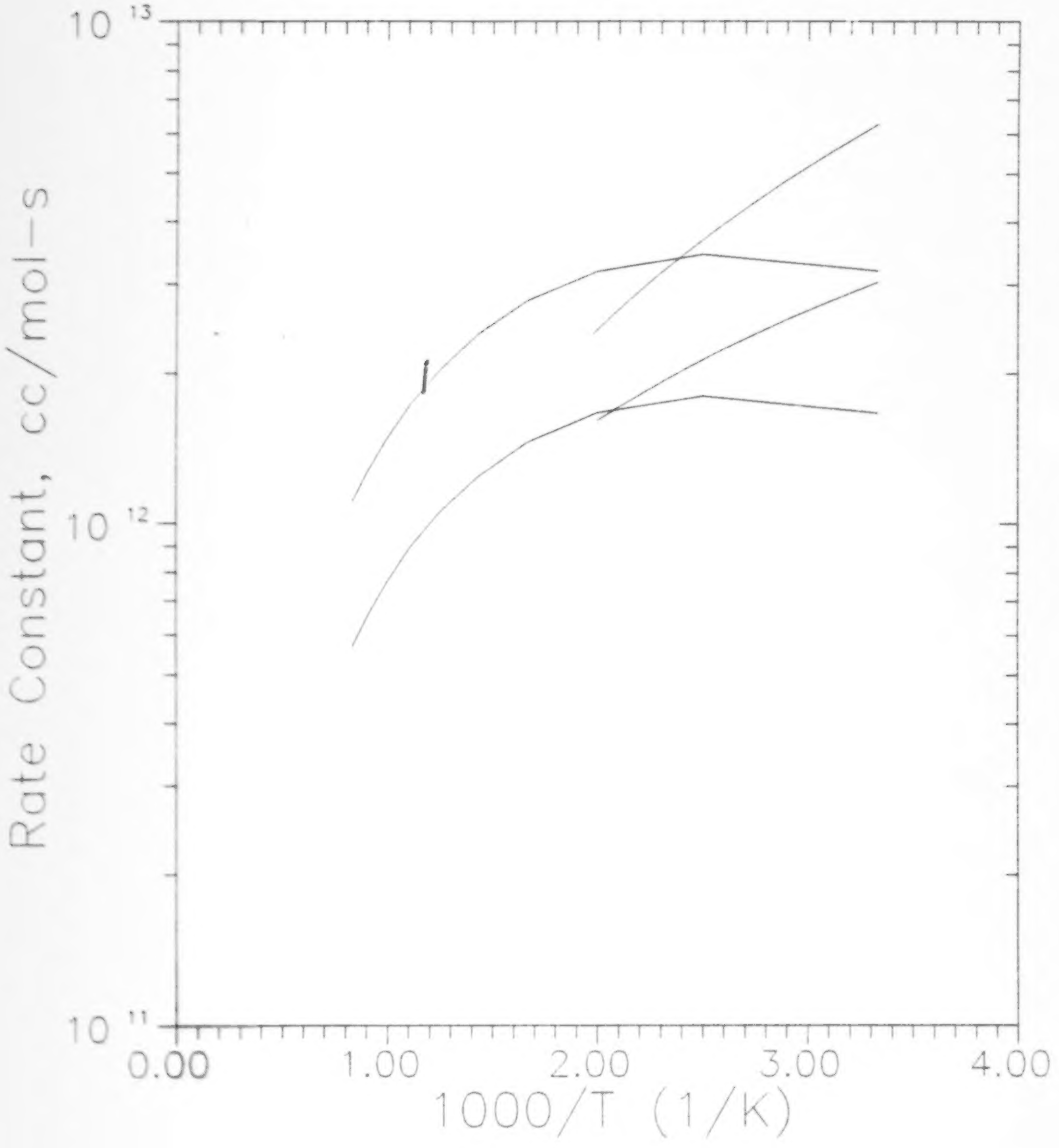
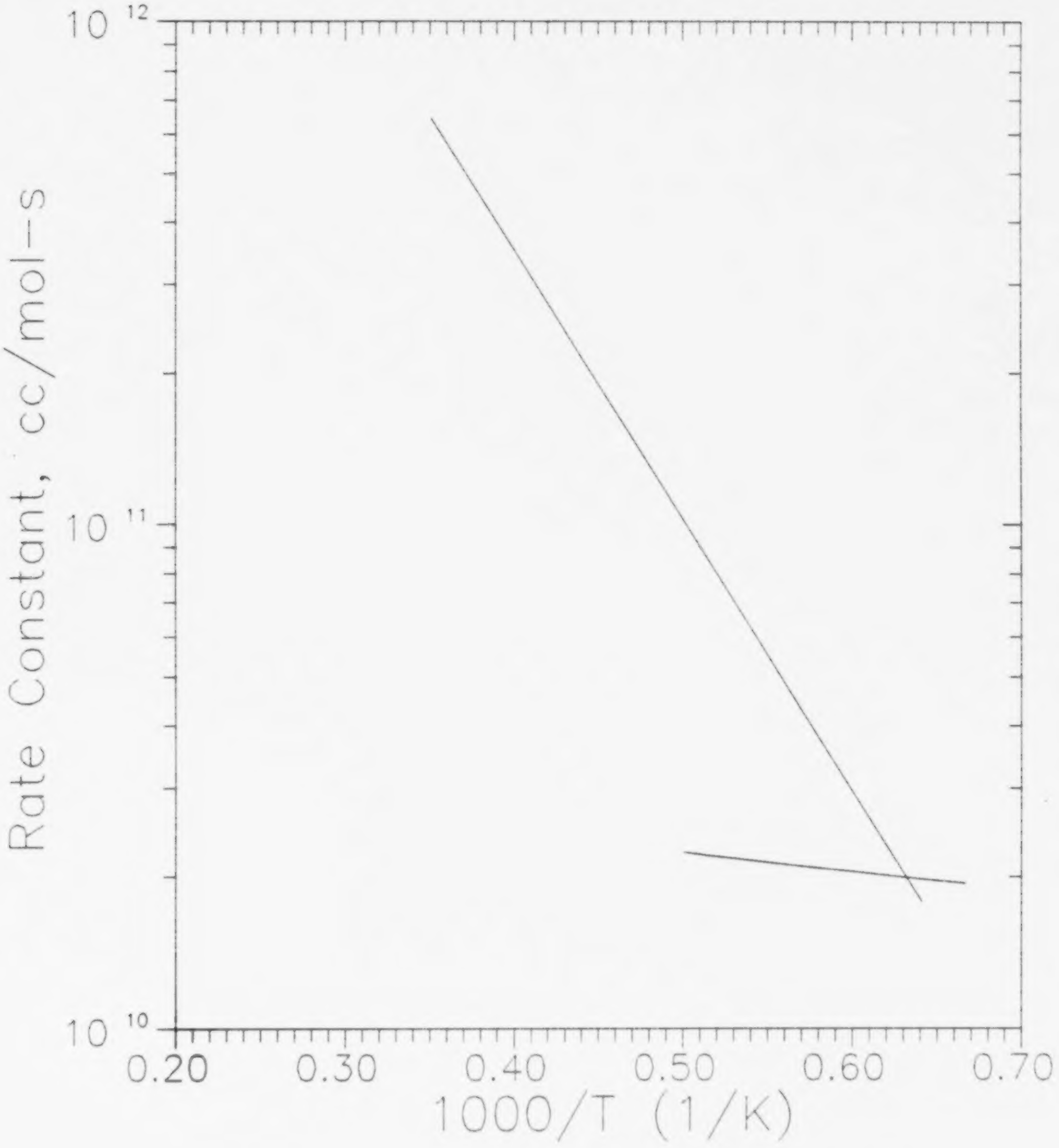
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH2 + NO = HN2 + HO**



10 13
10 12
10 11
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**NH2 + NO = N2 + H2O**



$10^{12}$
$10^{11}$
$10^{10}$
Rate Constant, cc/mol-s
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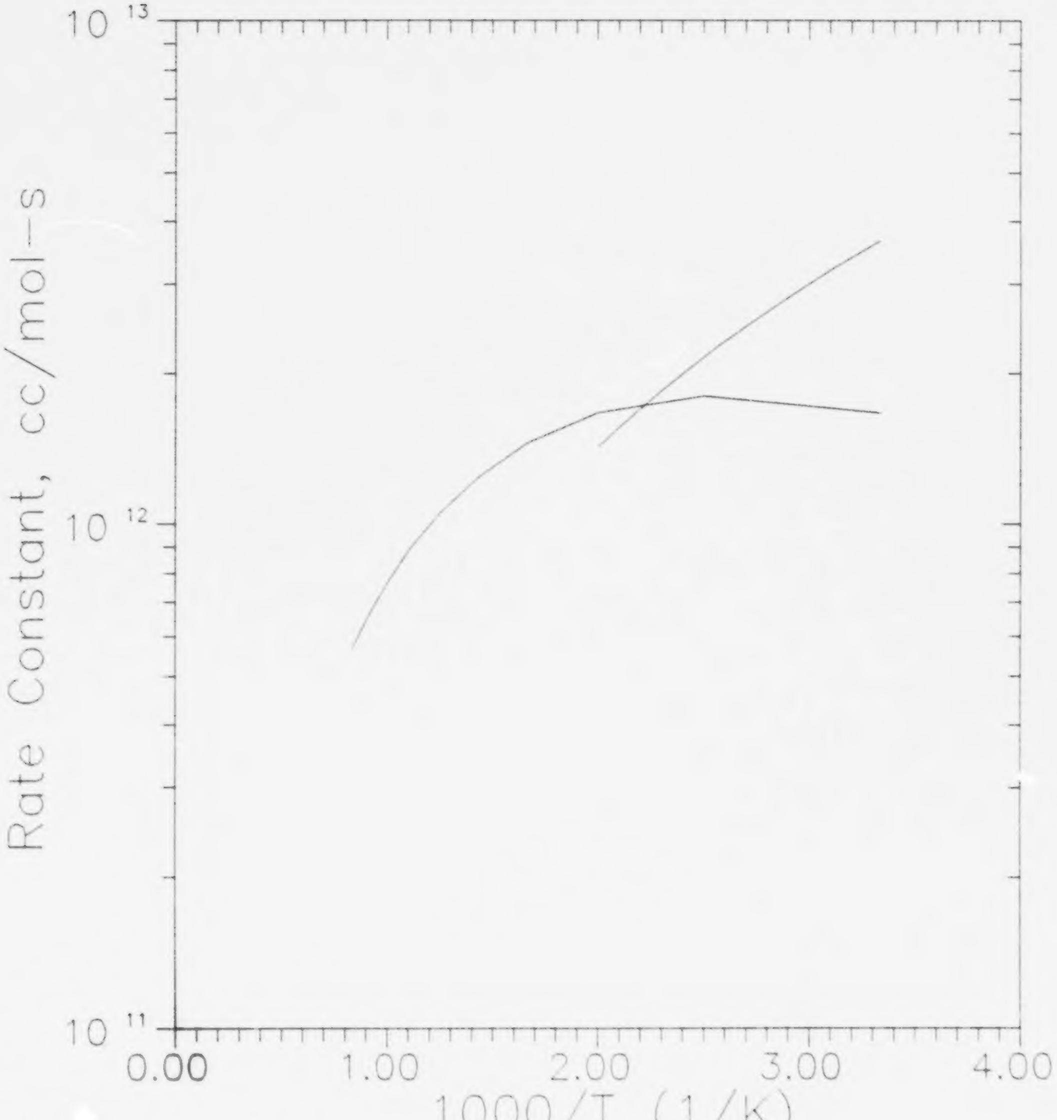
0.30
0.40
0.50
0.60
0.70
1000/T (1/K)

**NH2 + NO = N2O + H2**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10 12
10 11
Rate Constant, cc/mol-s
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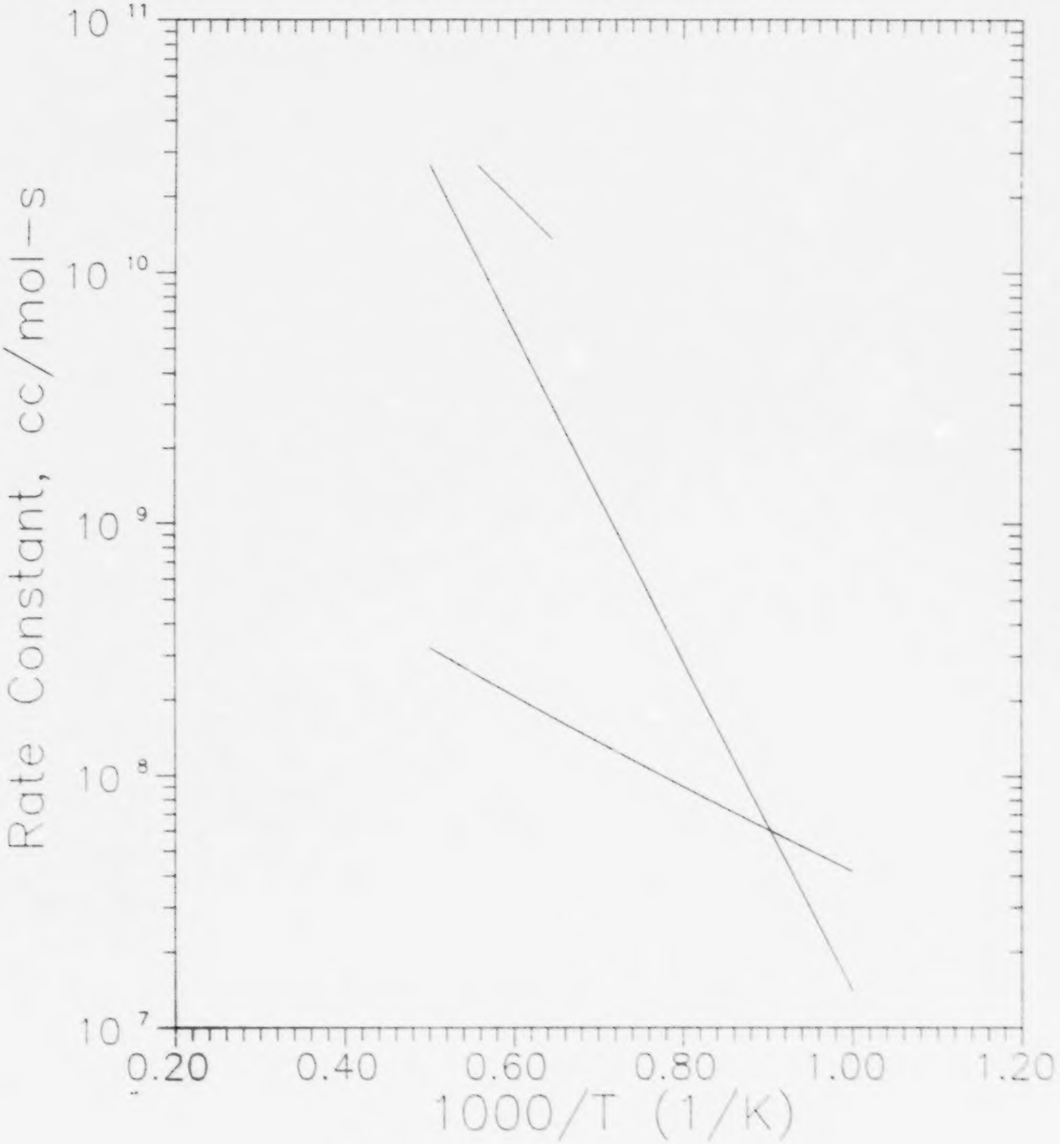
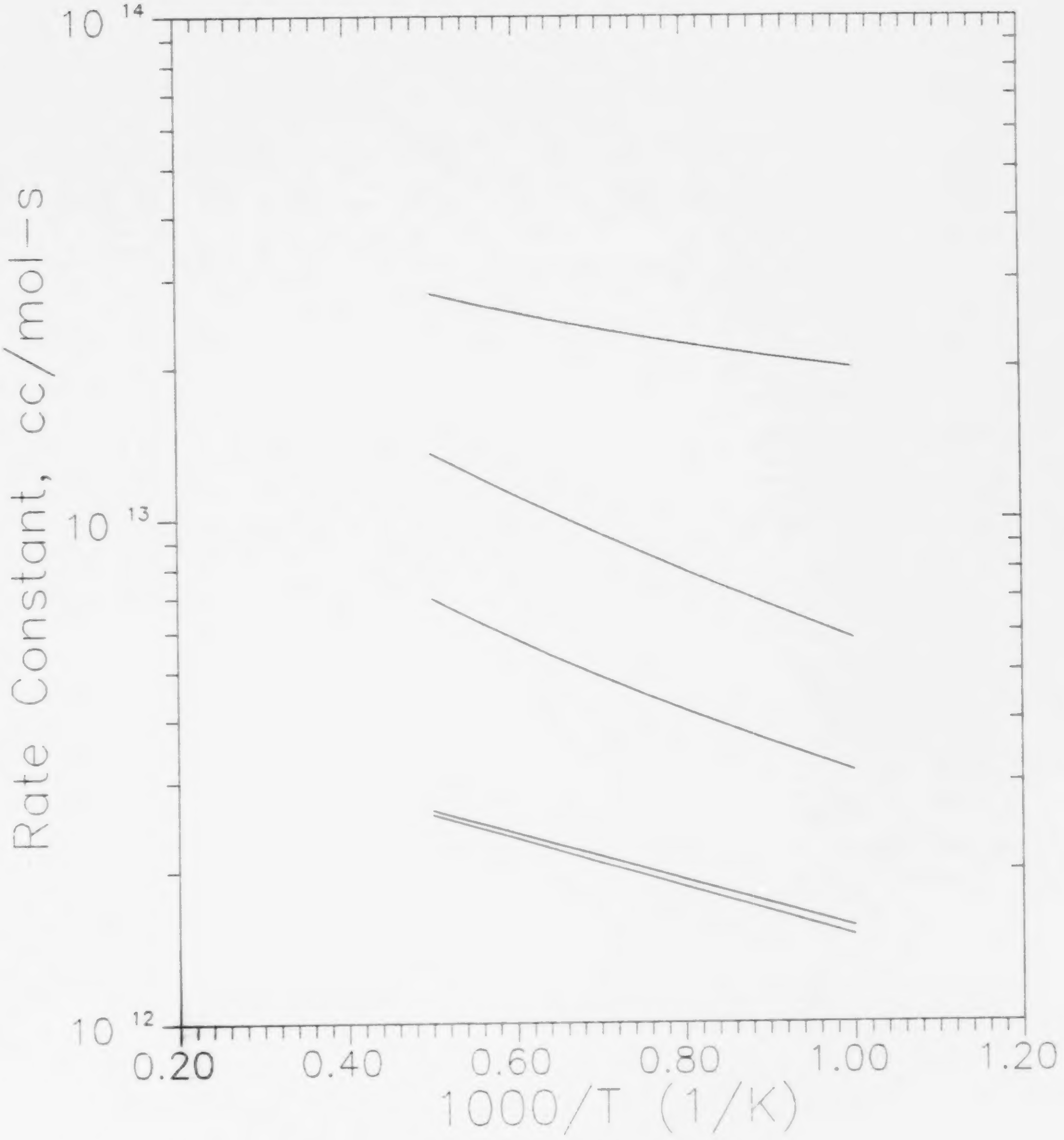
1.00
2.00
3.00
4.00
1000/T (1/K)

**NH2 + NO = N2 + H + HO**


Rate Constant, cc/mol-s
10 11
10 10
10 9
10 8
10 7
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH2 + O2 = HNO + HO**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10 13
10 12
Rate Constant, cc/mol-s
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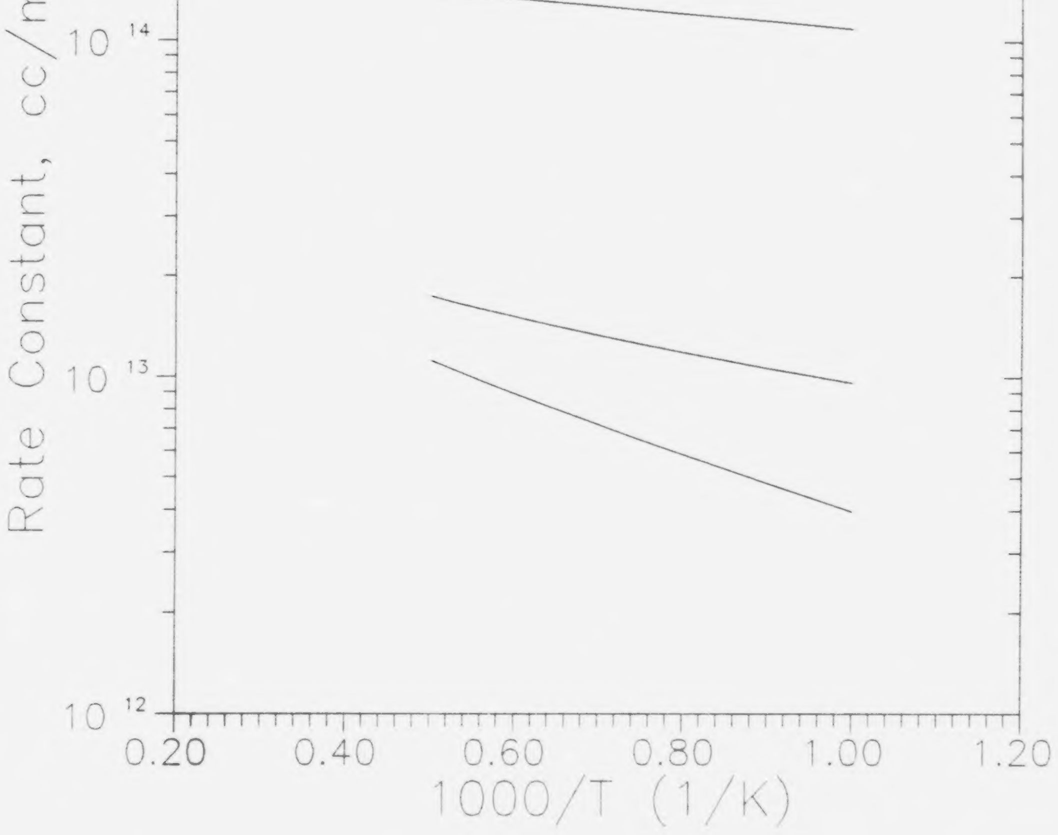
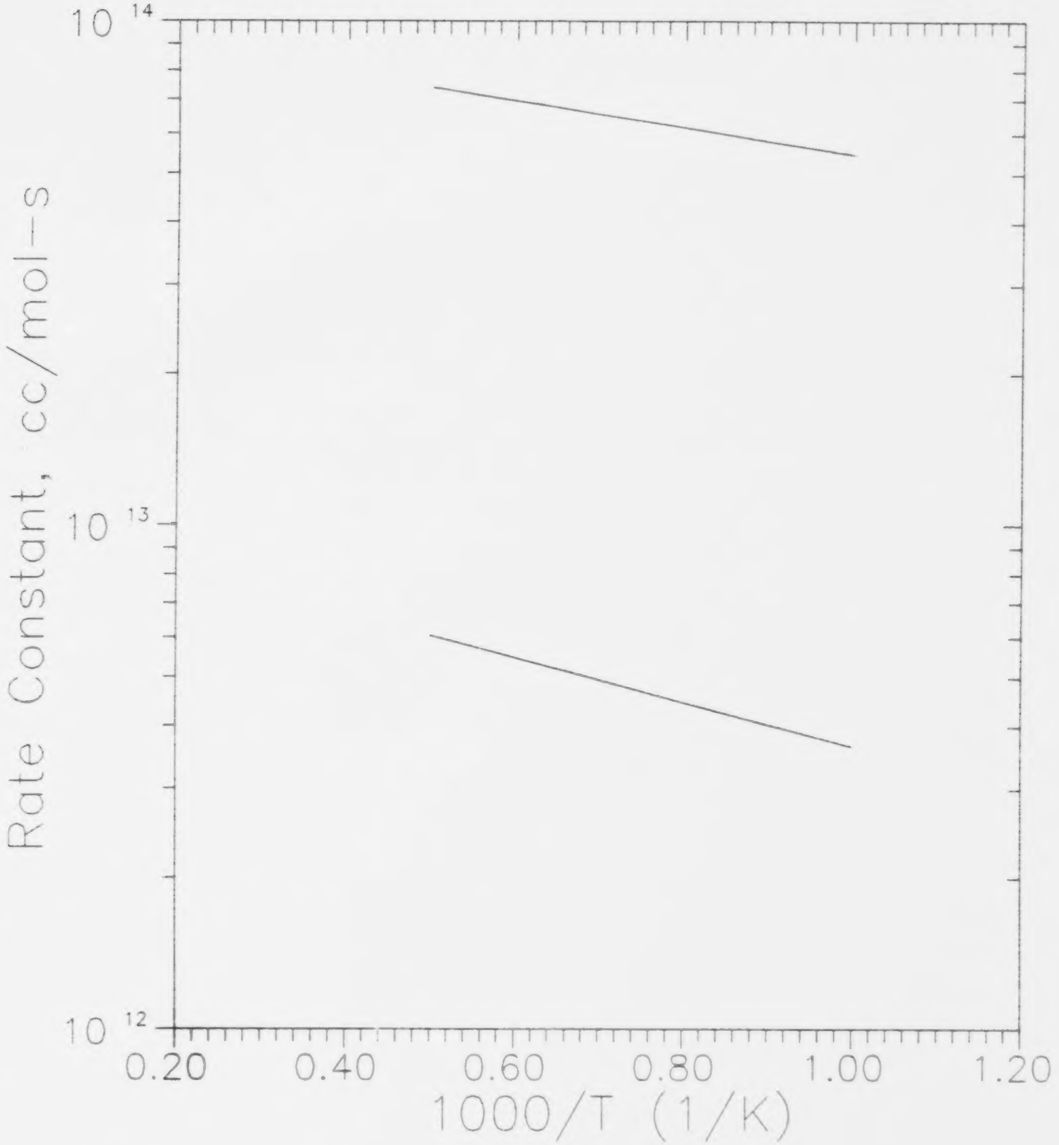
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

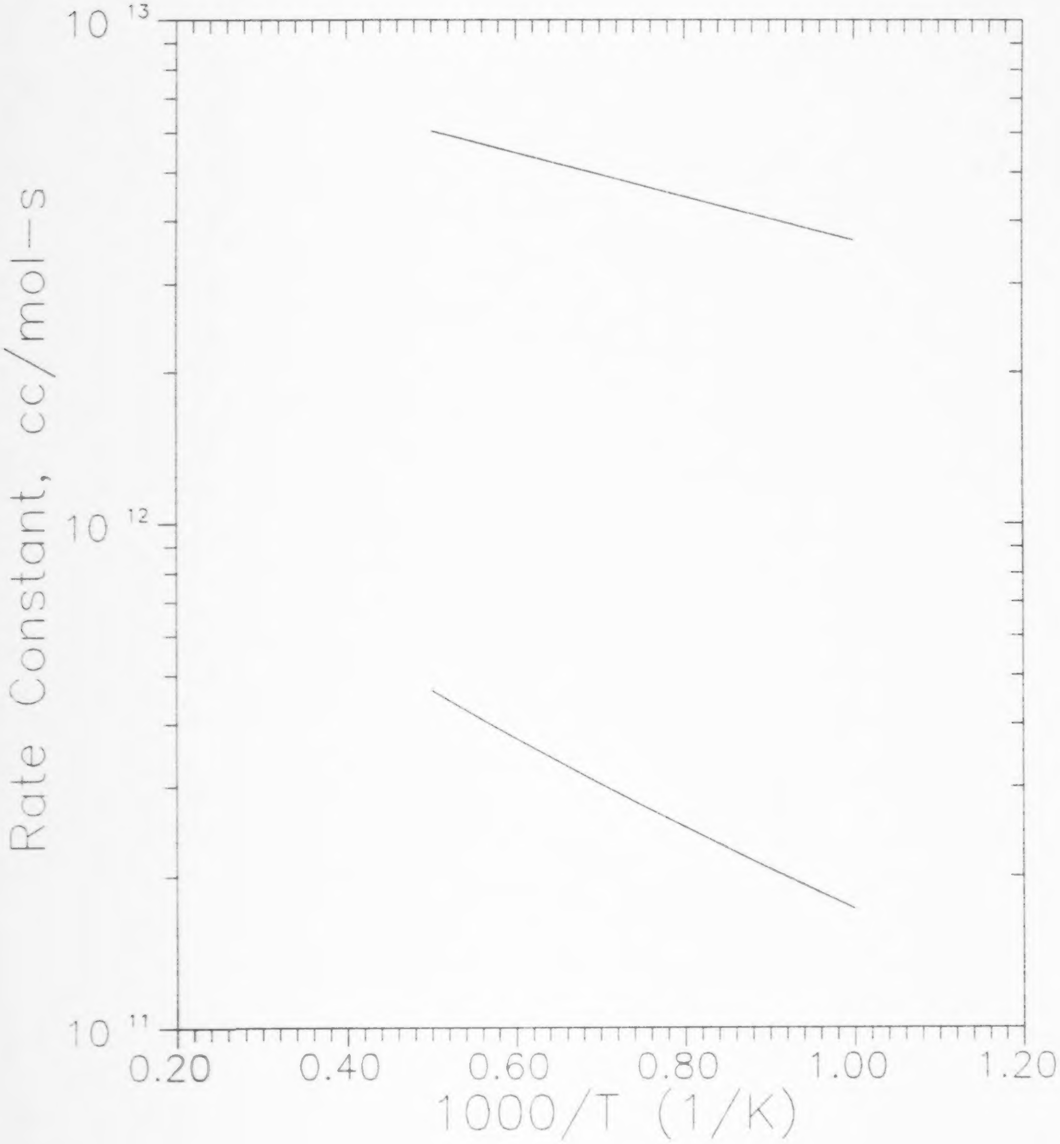
**NH2 + HO = NH + H2O**



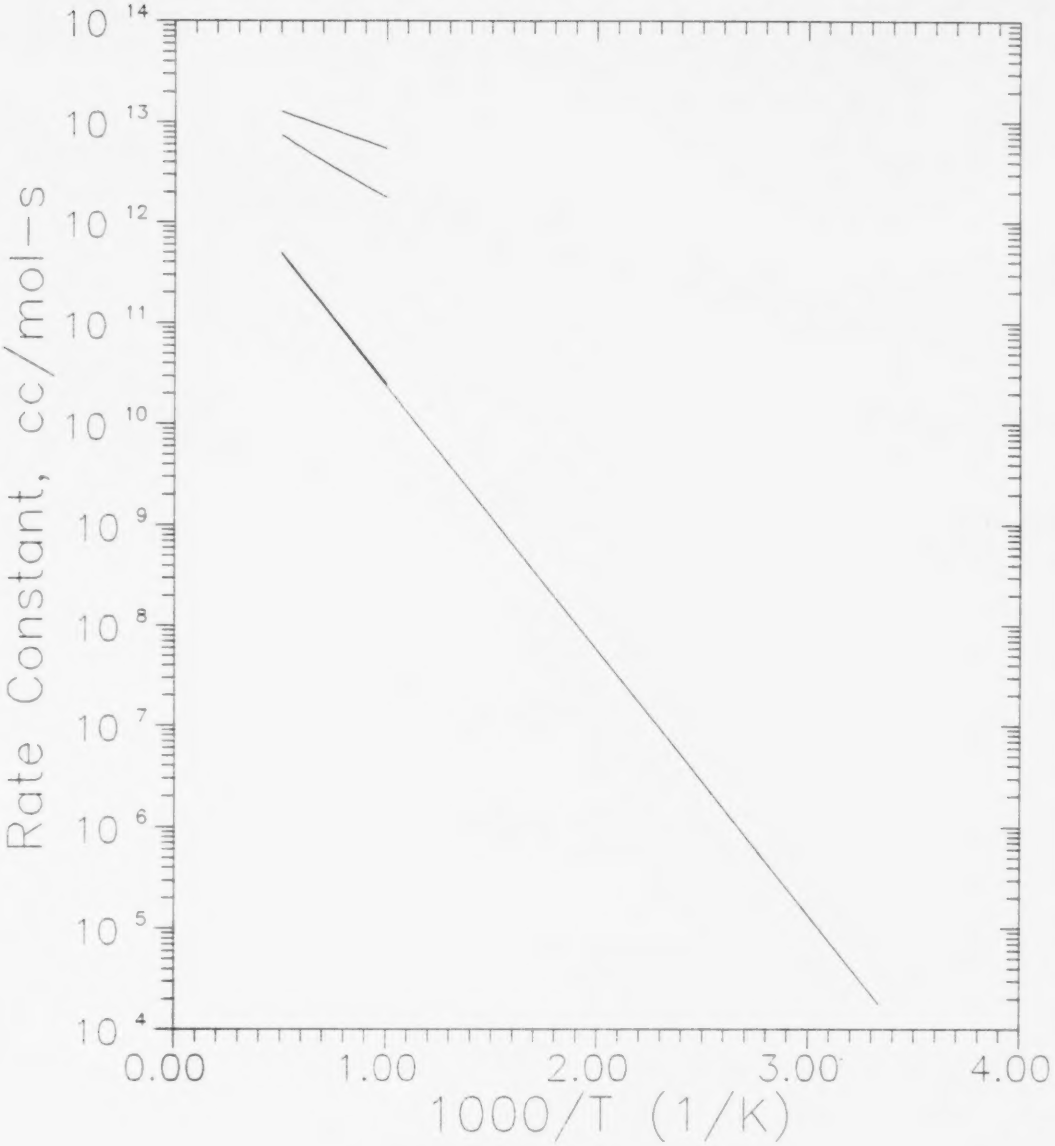
**NH2 + HNO = NH3 + NO**



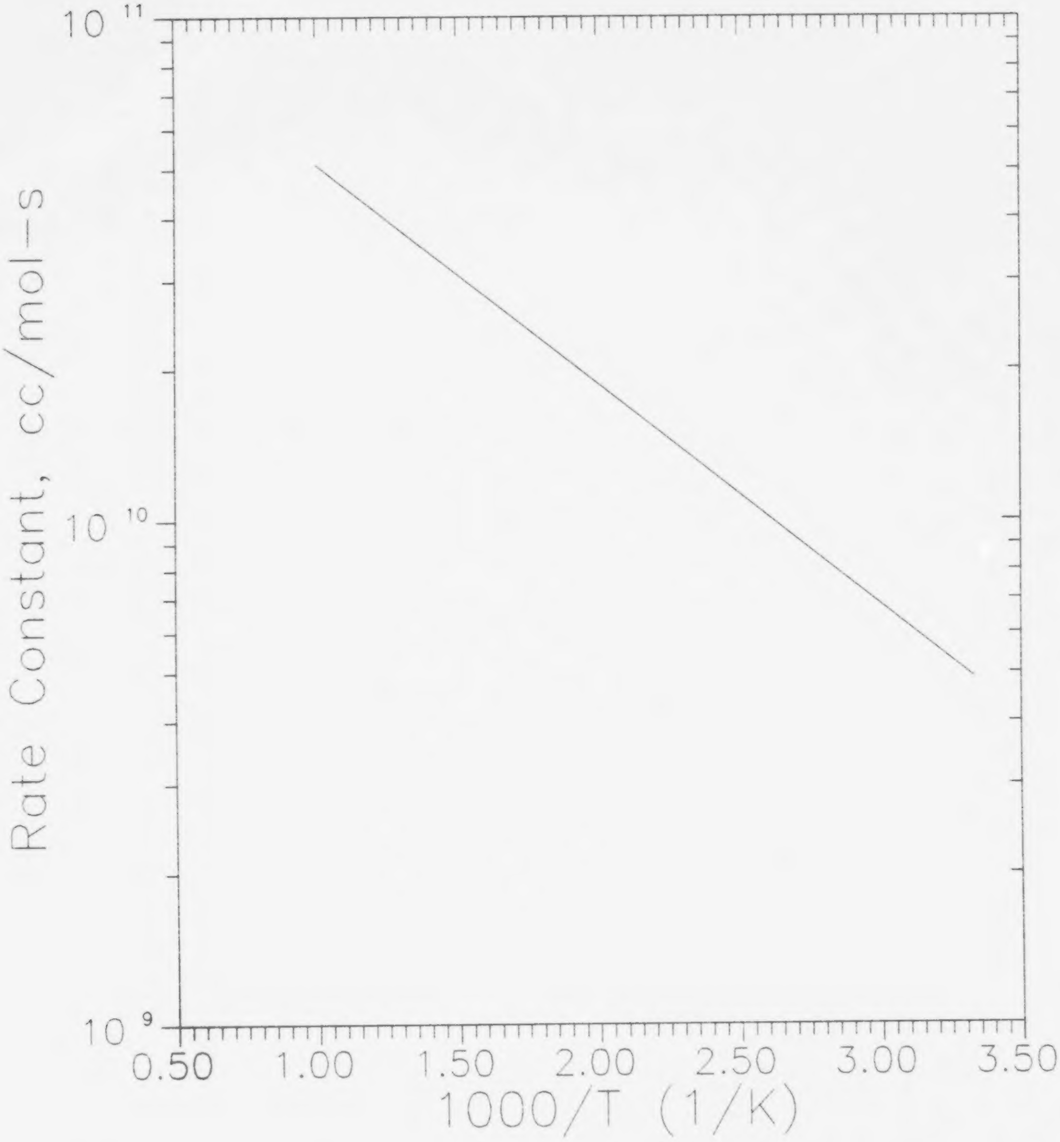
**NH2 + HO2 = NH + H2O2**



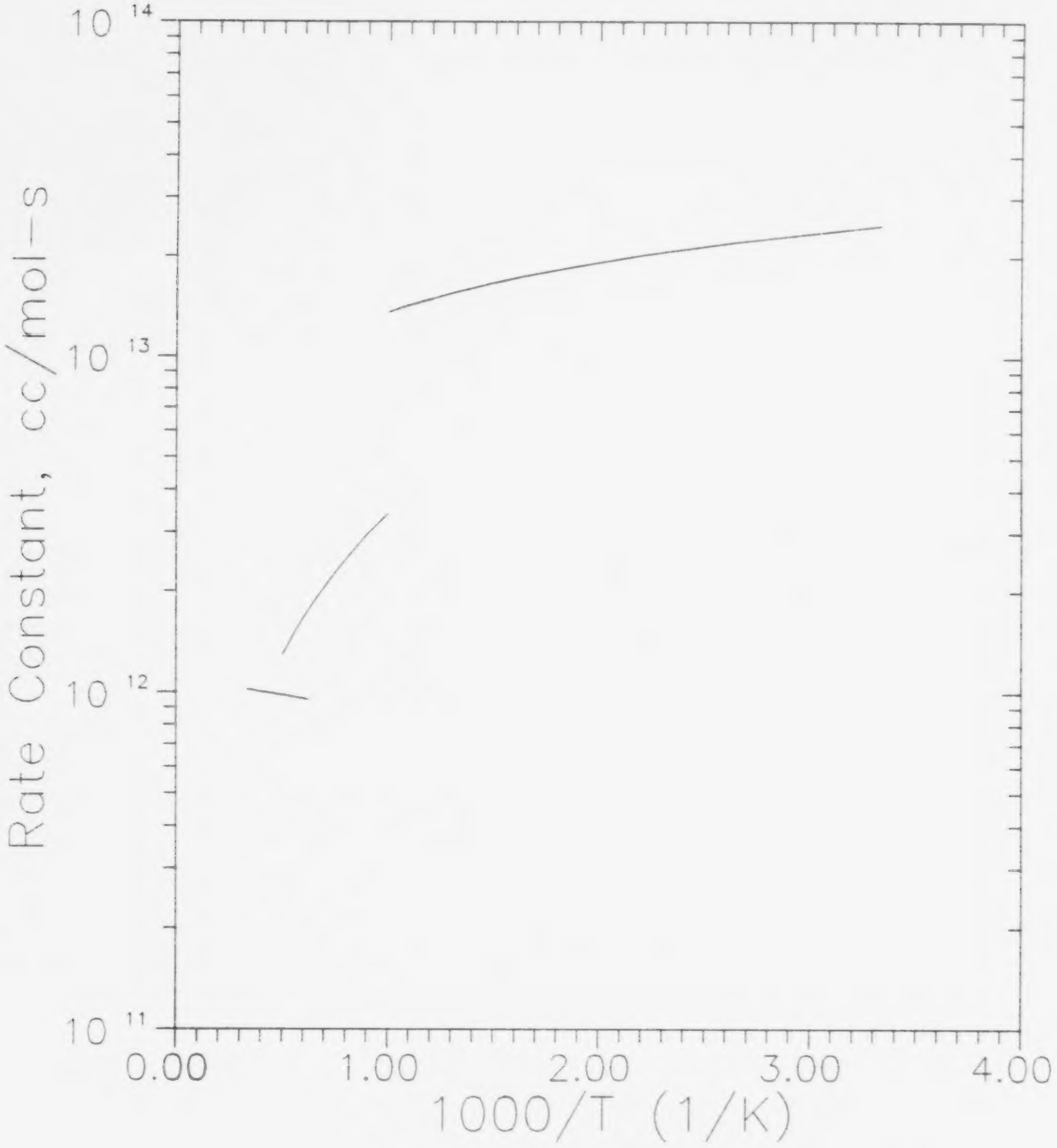
**NH2 + HO2 = NH3 + O2**


10 14
10 13
10 12
10 11
10 10
10 9
10 8
10 7
10 6
10 5
10 4
Rate Constant, cc/mol-s
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

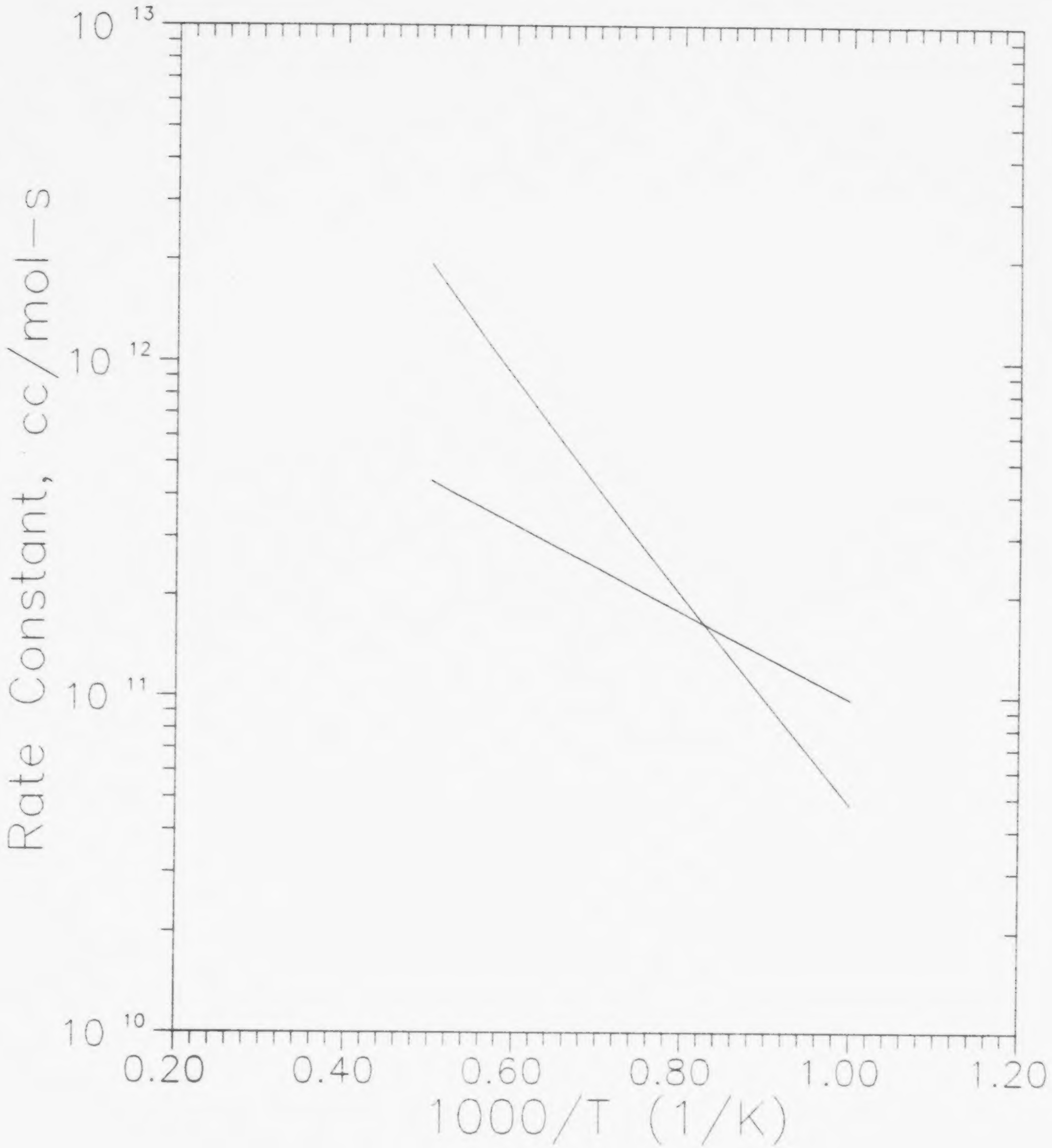
**NH + O2 = HNO + O**


10 ¹¹
10 ¹⁰
10 ⁹
Rate Constant, cc/mol-s
0.50
1.00
1.50
2.00
2.50
3.00
3.50
1000/T (1/K)

**NH + O2 = NO + HO**


Rate Constant, cc/mol-s
10 ¹⁴
10 ¹³
10 ¹²
10 ¹¹
0.00
1.00
2.00
3.00
4.00
1000/T (1/K)

**NH + NO = N2O + H**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$10^{12}$
$10^{11}$
$10^{10}$
Rate Constant, cc/mol-s
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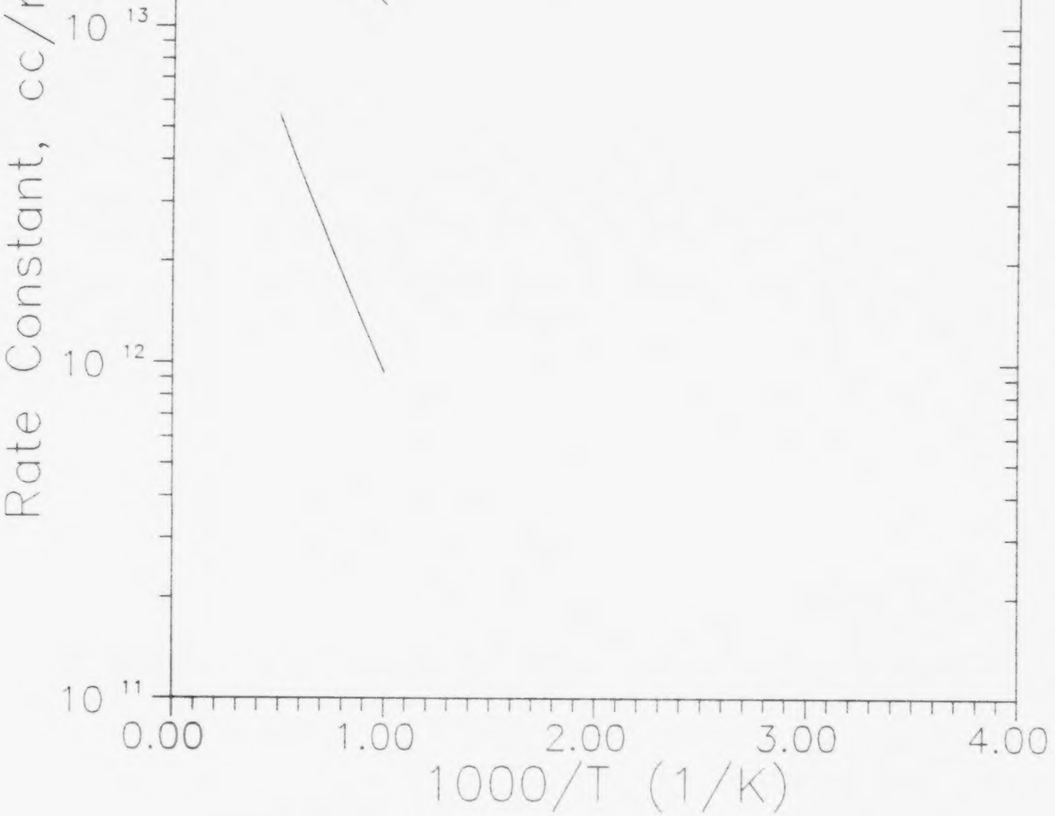
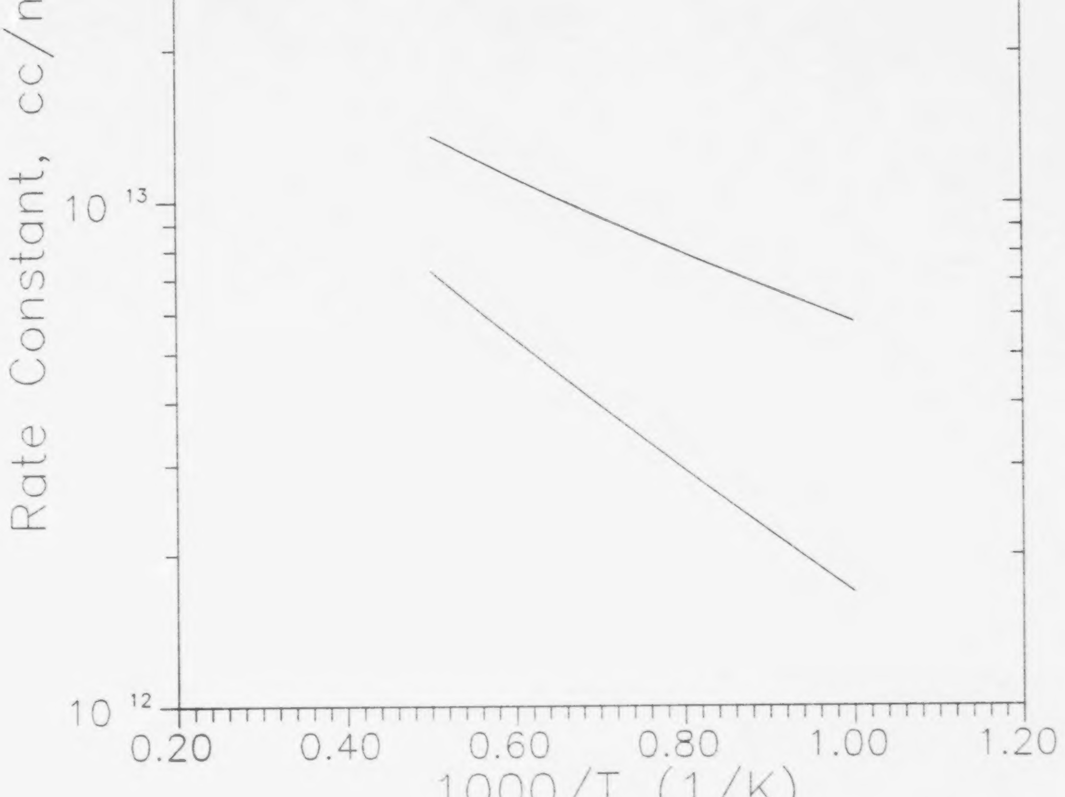
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

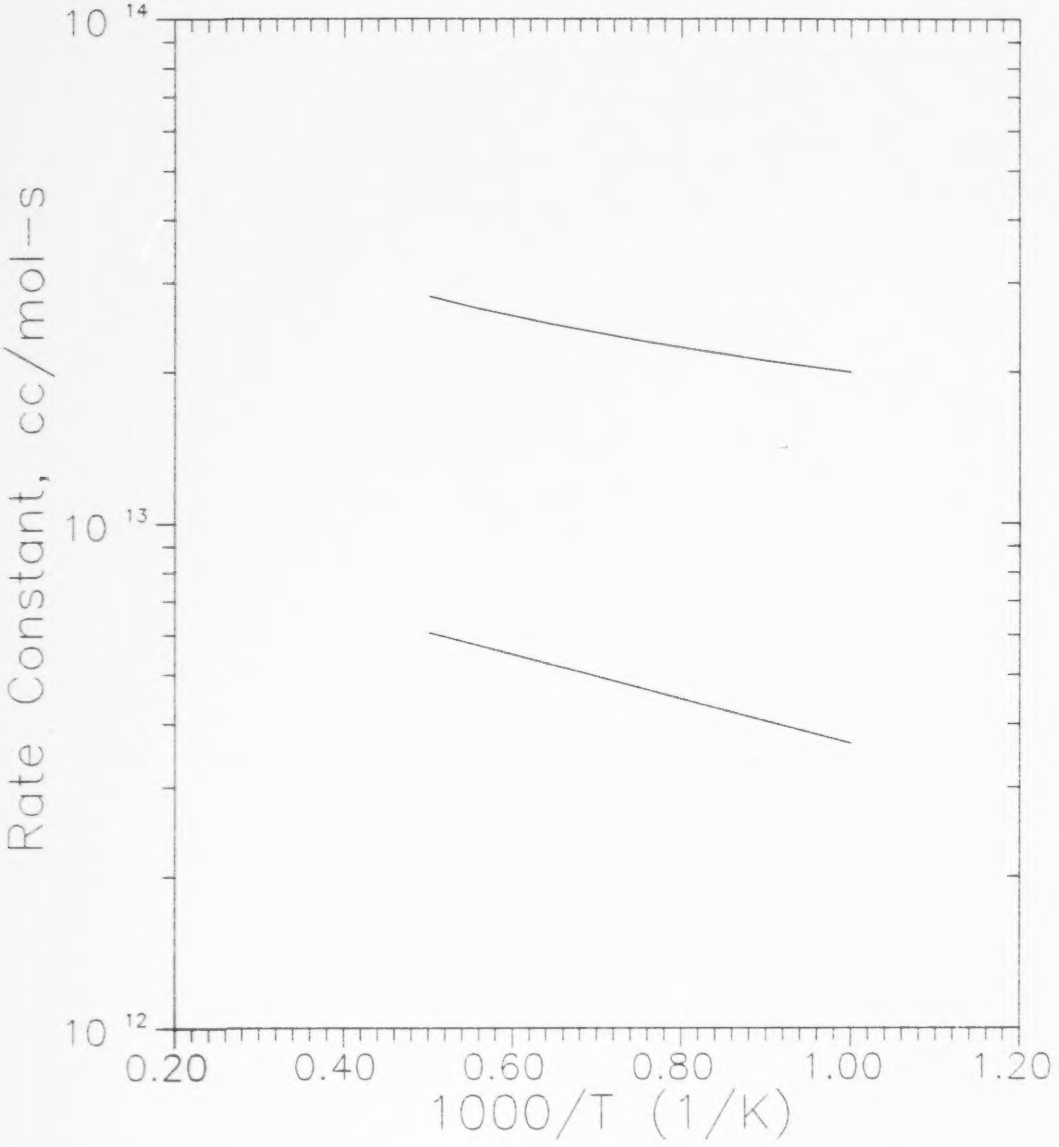
**NH + N2O = N2 + HNO**



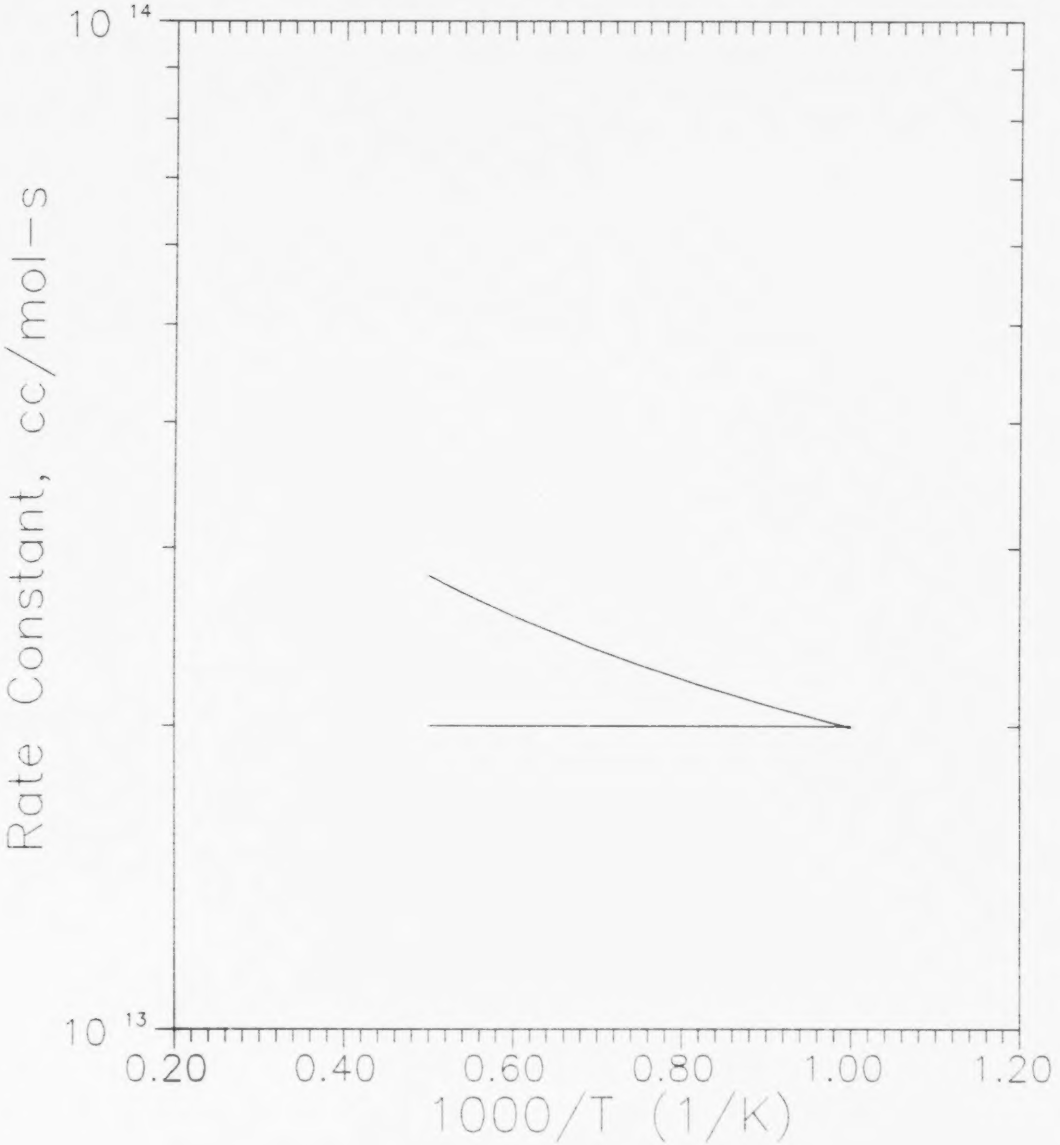
**$NH \quad + HO \qquad = HNO \quad + H$**


Rate Constant, cc/mol-s
10 14
10 13
10 12
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

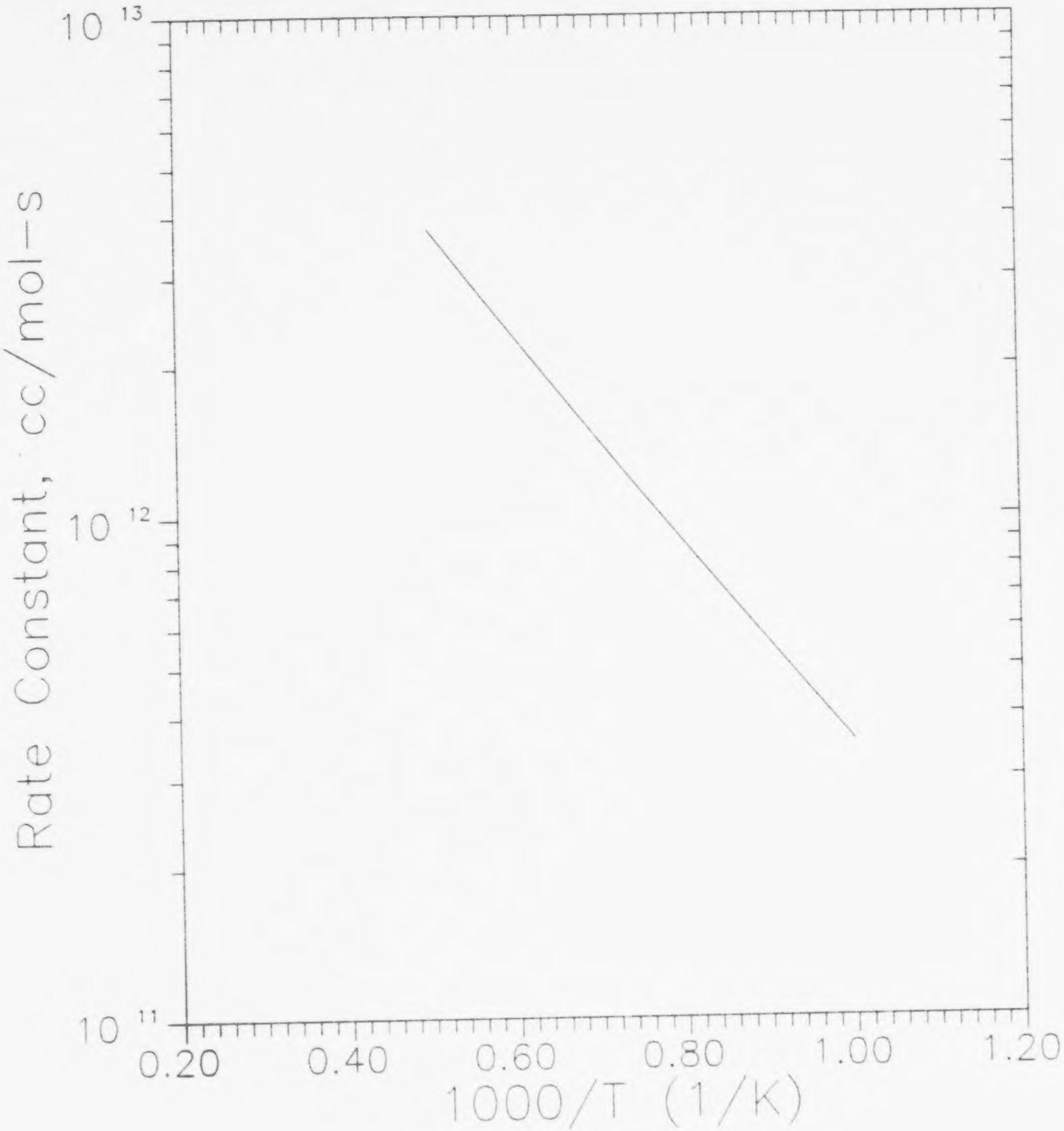
**NH + HO = N + H2O**


10 ¹⁴
10 ¹³
10 ¹²
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH + HO2 = HNO + HO**


10 14
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH + O = NO + H**



10 13
10 12
10 11
Rate Constant, cc/mol-s
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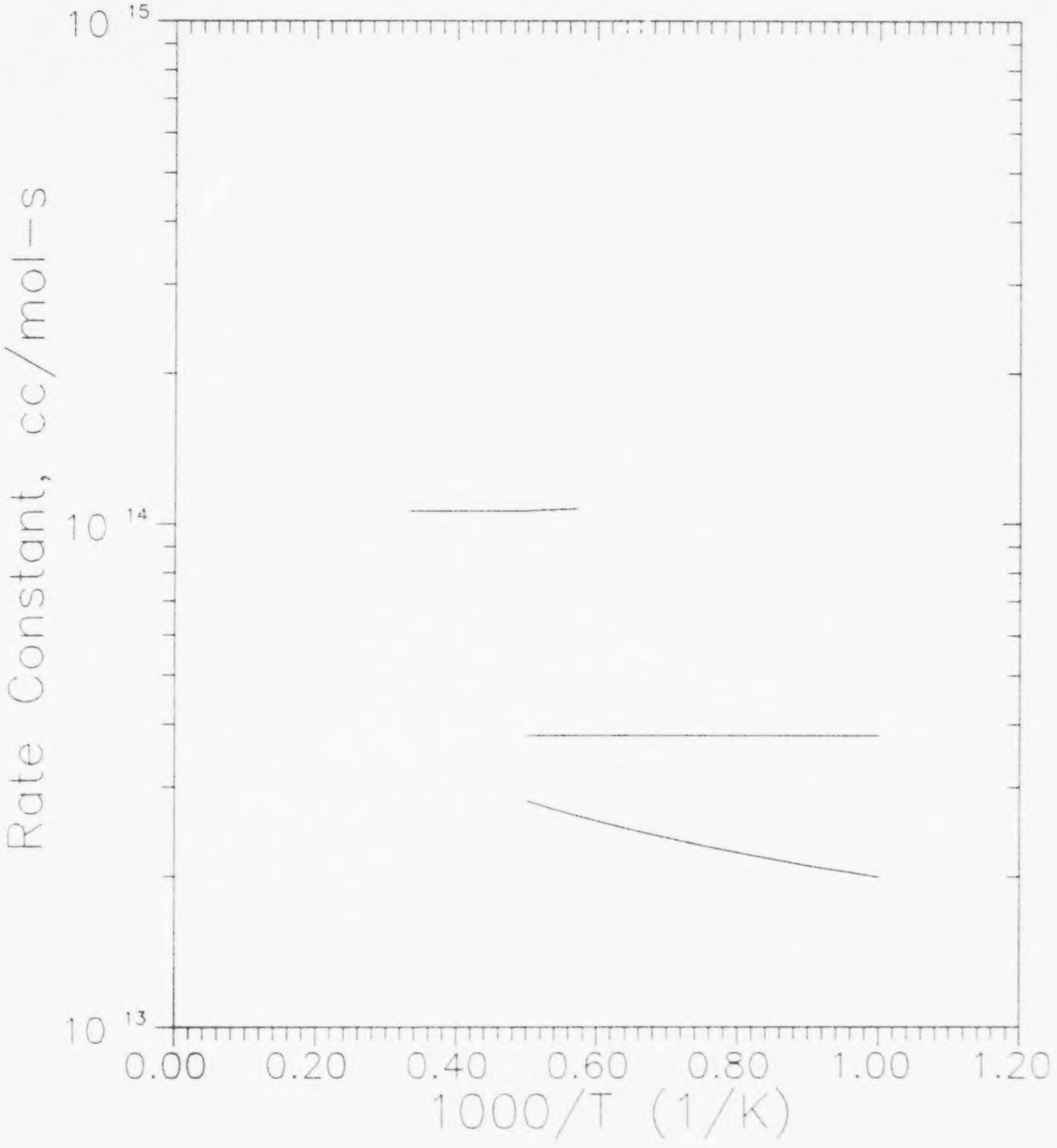
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NH + O = N + HO**


Rate Constant, cc/mol-s
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$10^{14}$
$10^{13}$
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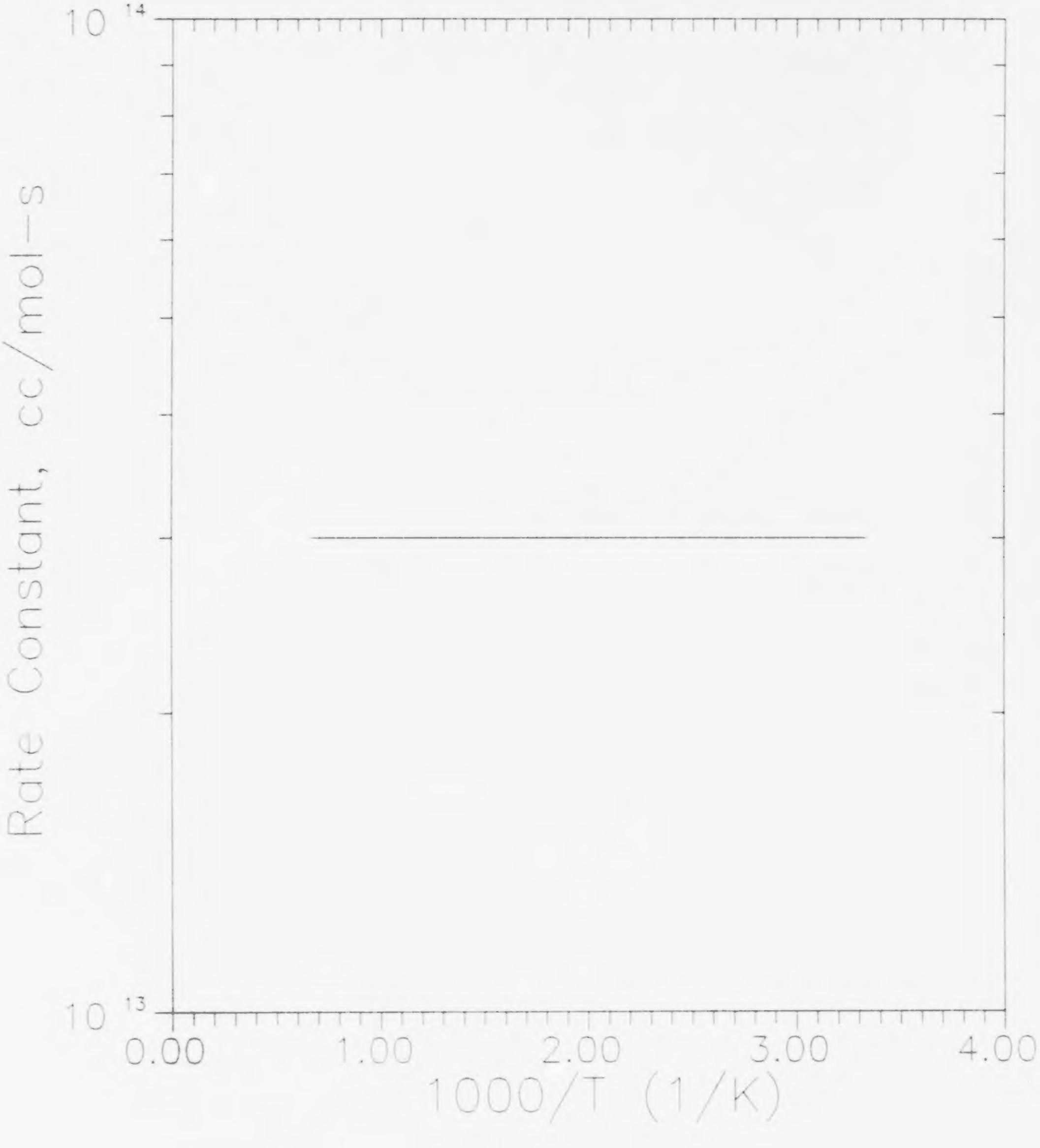
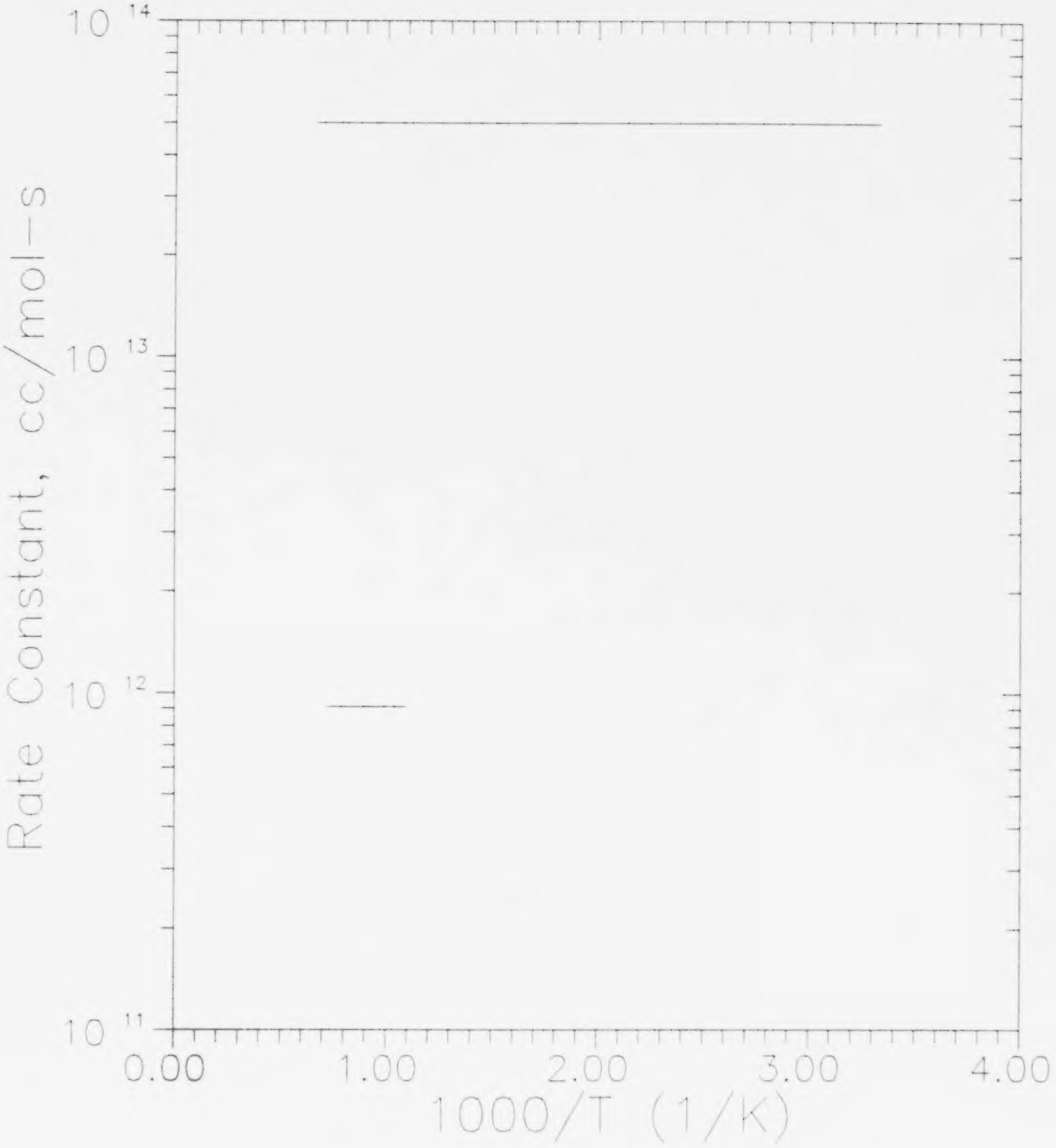
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**N + HO = NO + H**



**HN2 + HO = N2 + H2O**


$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
Rate Constant, cc/mol-s
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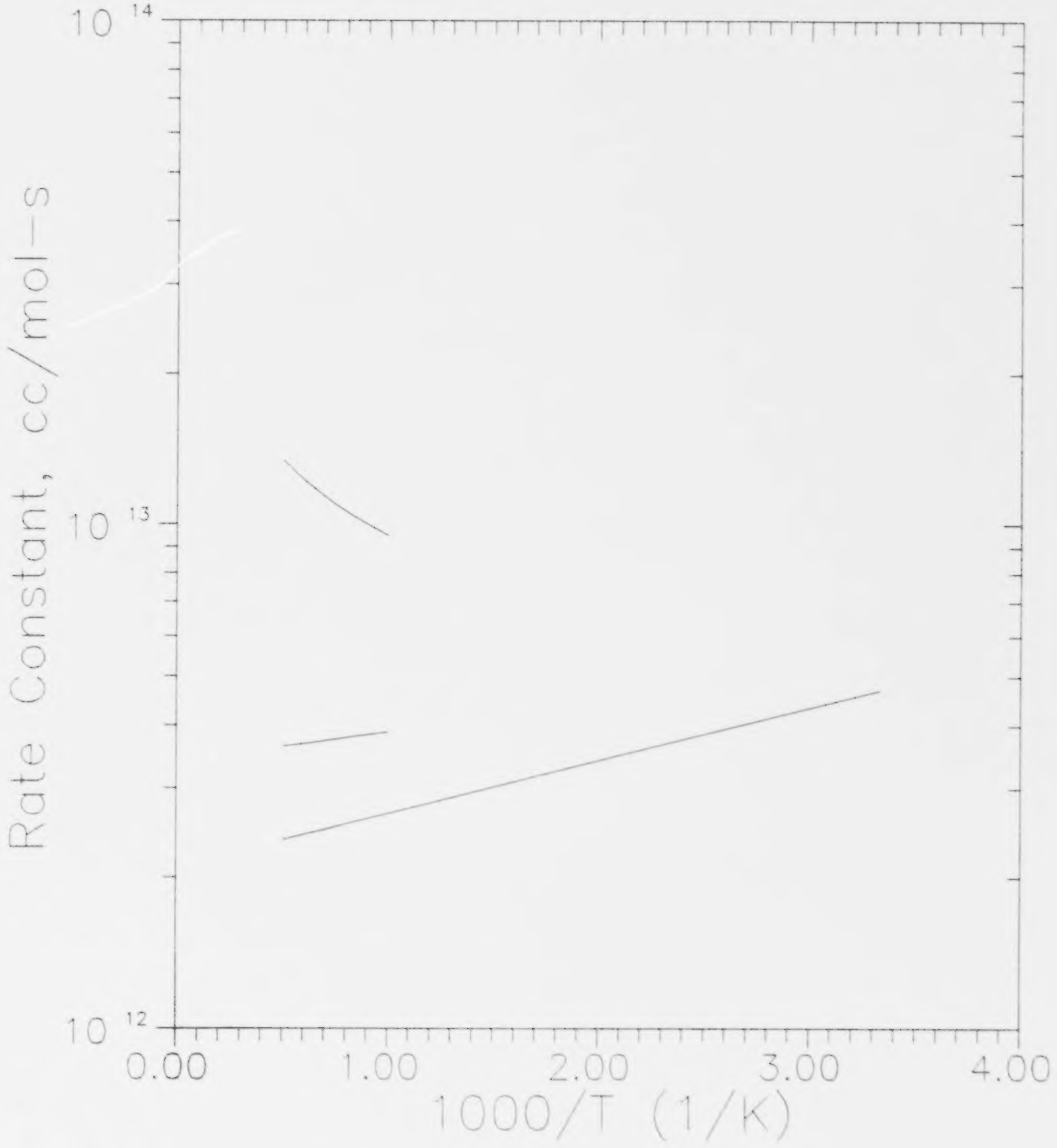
1.00
2.00
3.00
4.00
1000/T (1/K)

**HN2 + NO = N2 + HNO**



Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
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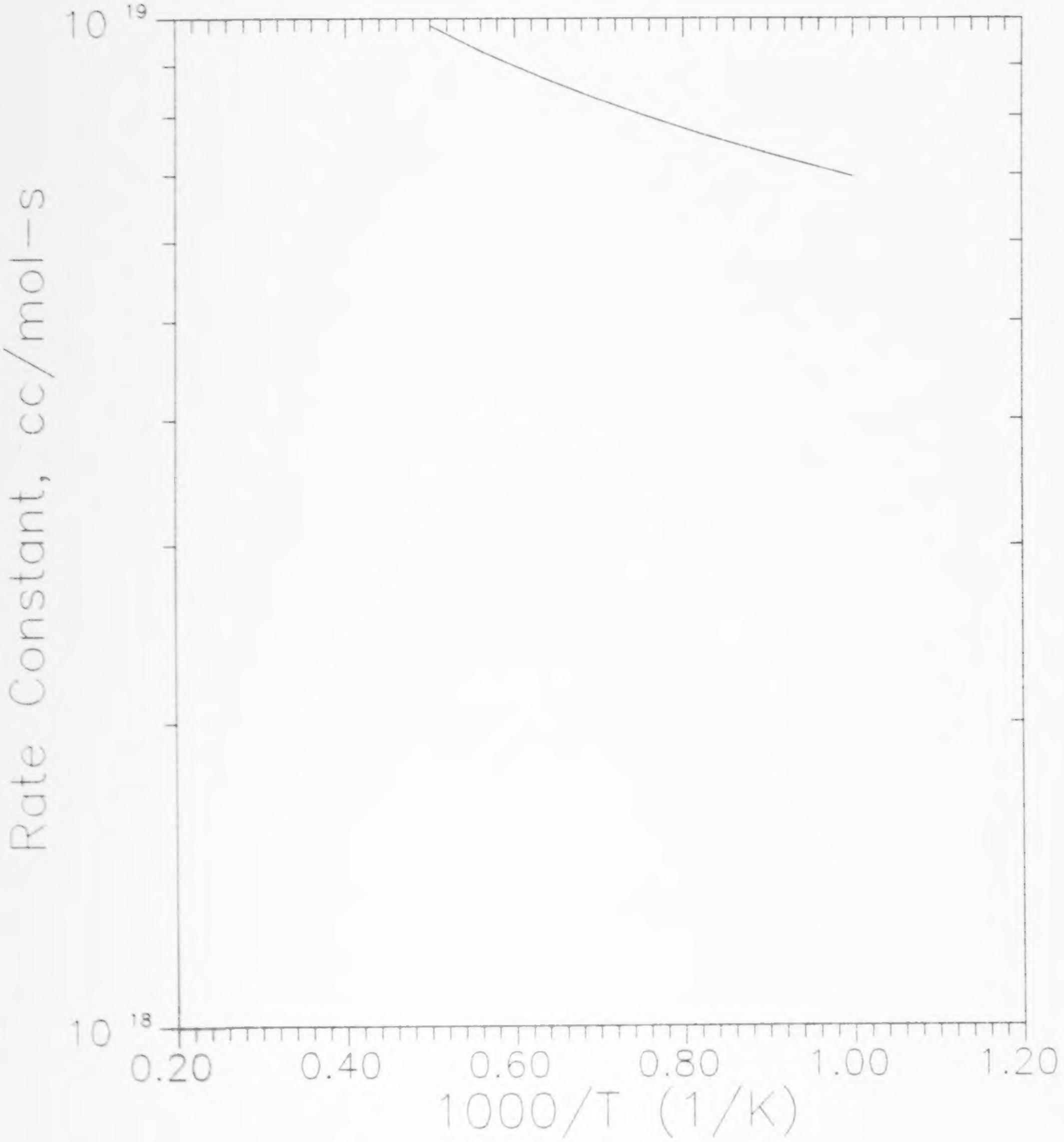
1.00
2.00
3.00
4.00
1000/T (1/K)

**NO + HO2 = NO2 + HO**



Rate Constant, cc/mol-s
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10^18
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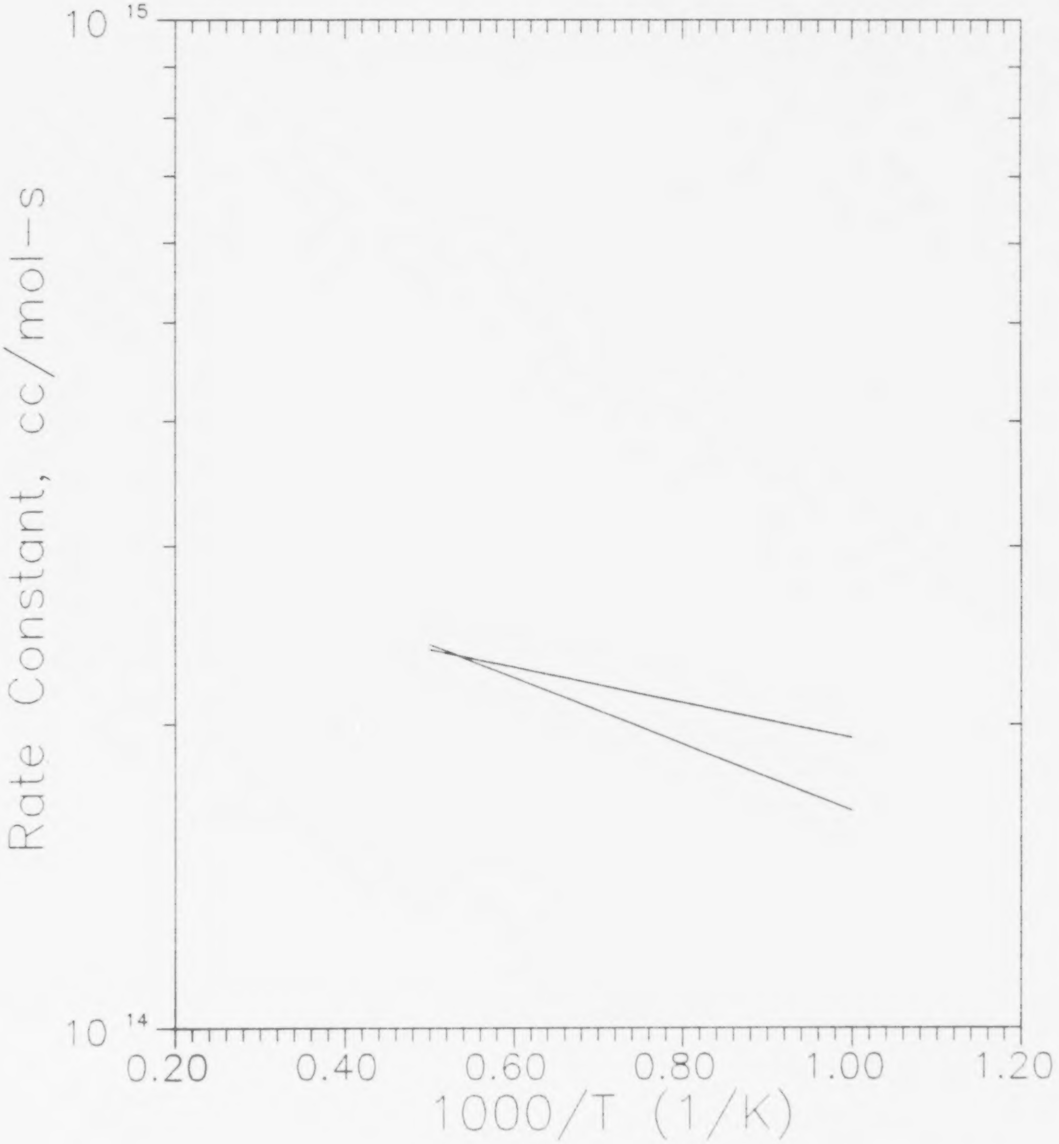
0.60
0.80
1.00
1.20
1000/T (1/K)

**NO + H + M = HNO + M**


10 15
10 14
Rate Constant, cc/mol-s
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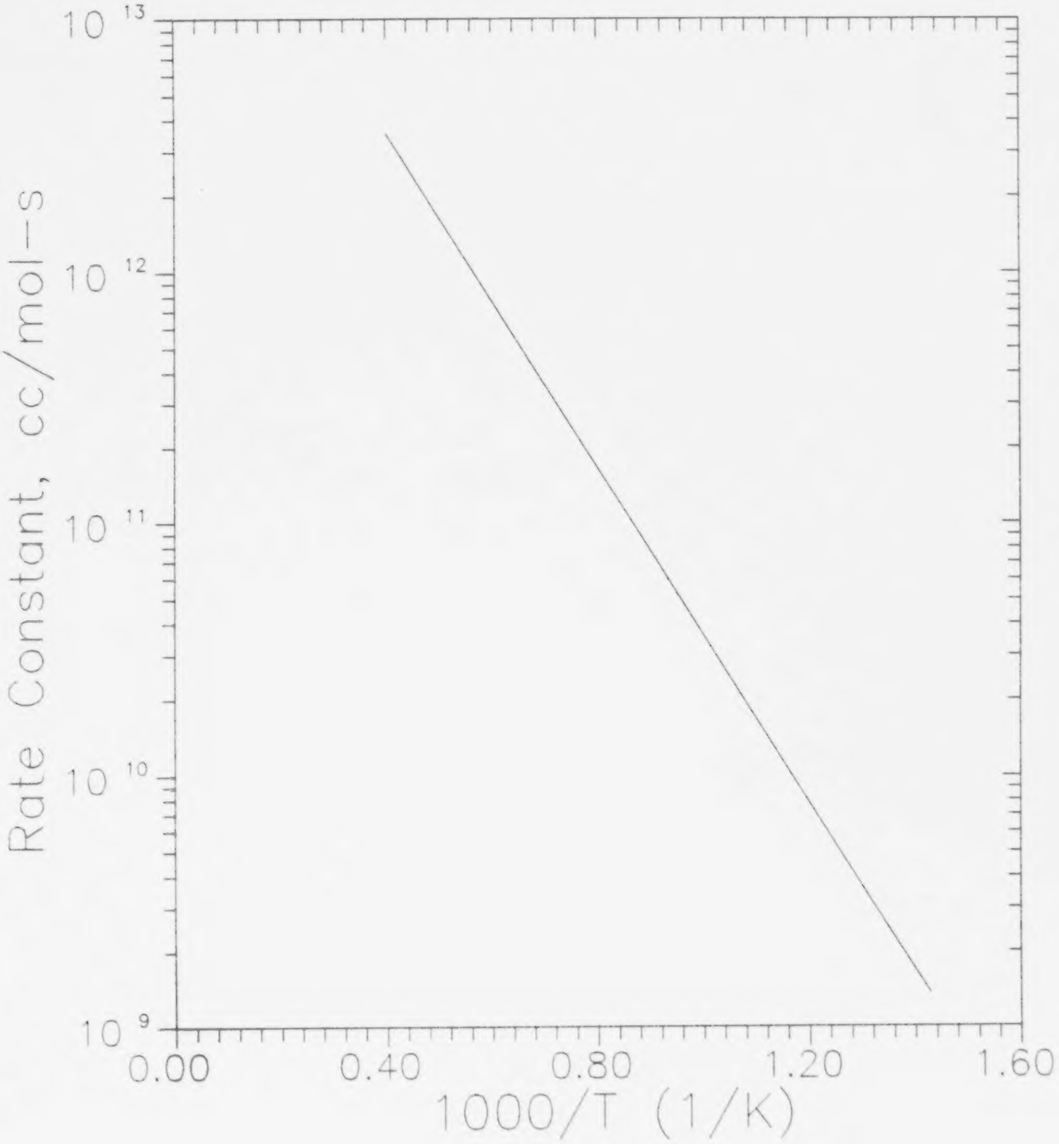
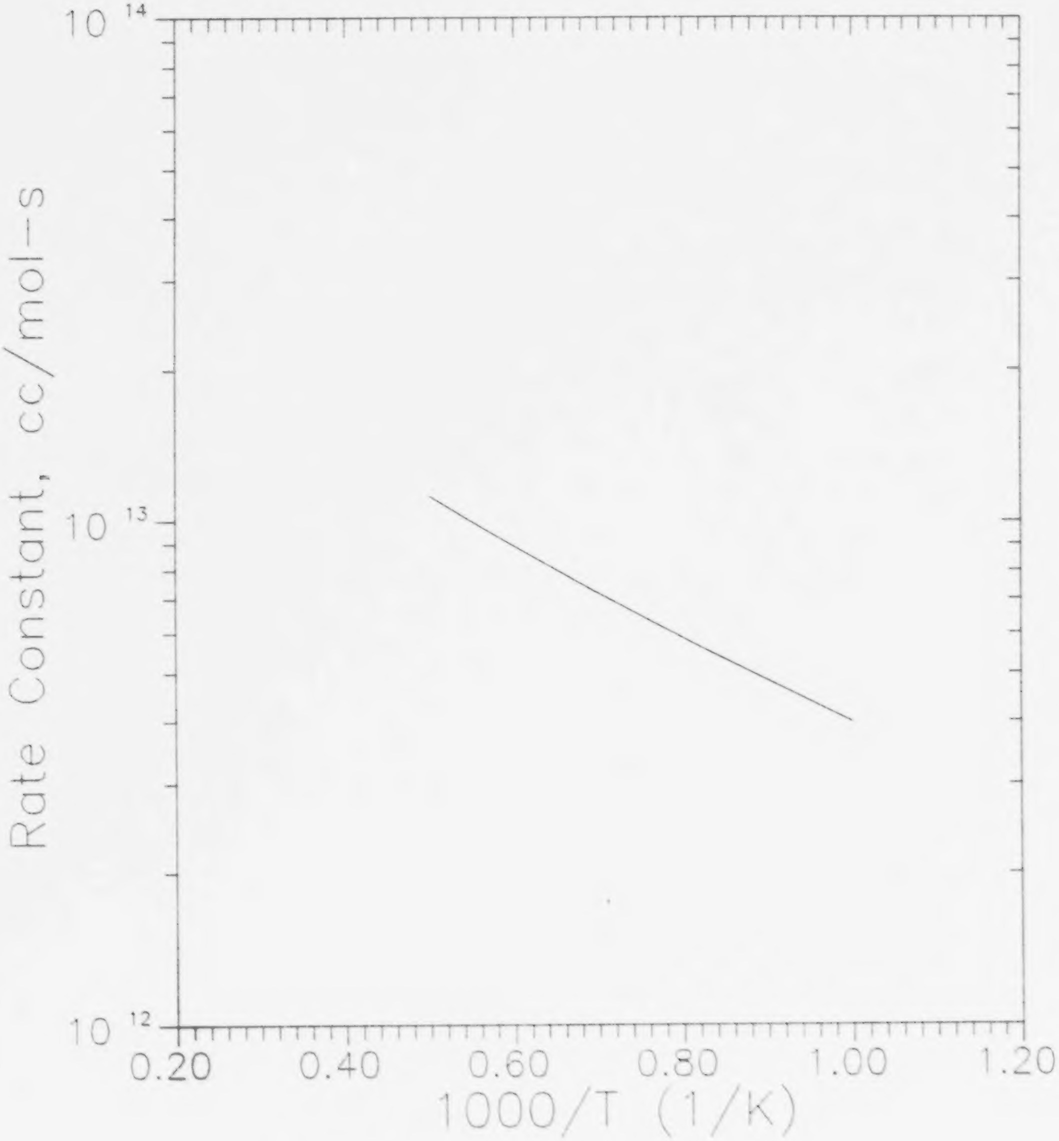
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NO2 + H = NO + HO**



10^13
10^12
10^11
10^10
10^9
Rate Constant, cc/mol-s
0.00
0.40
0.80
1.20
1.60
1000/T (1/K)

**N2O + H = N2 + HO**


10 14
10 13
10 12
Rate Constant, cc/mol−s
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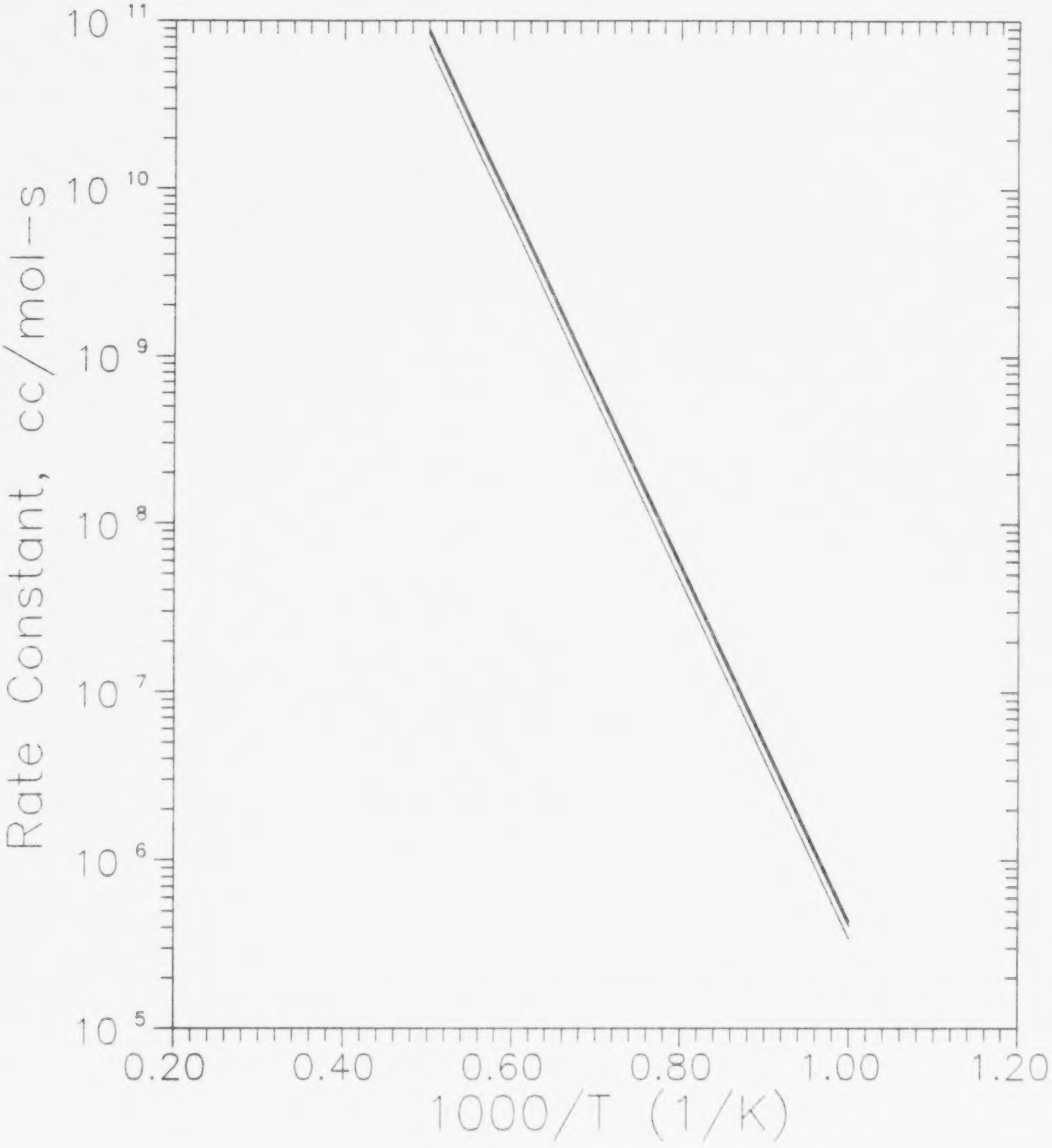
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HNO + O = HO + NO**



Rate Constant, cc/mol-s
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$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
$10^{5}$
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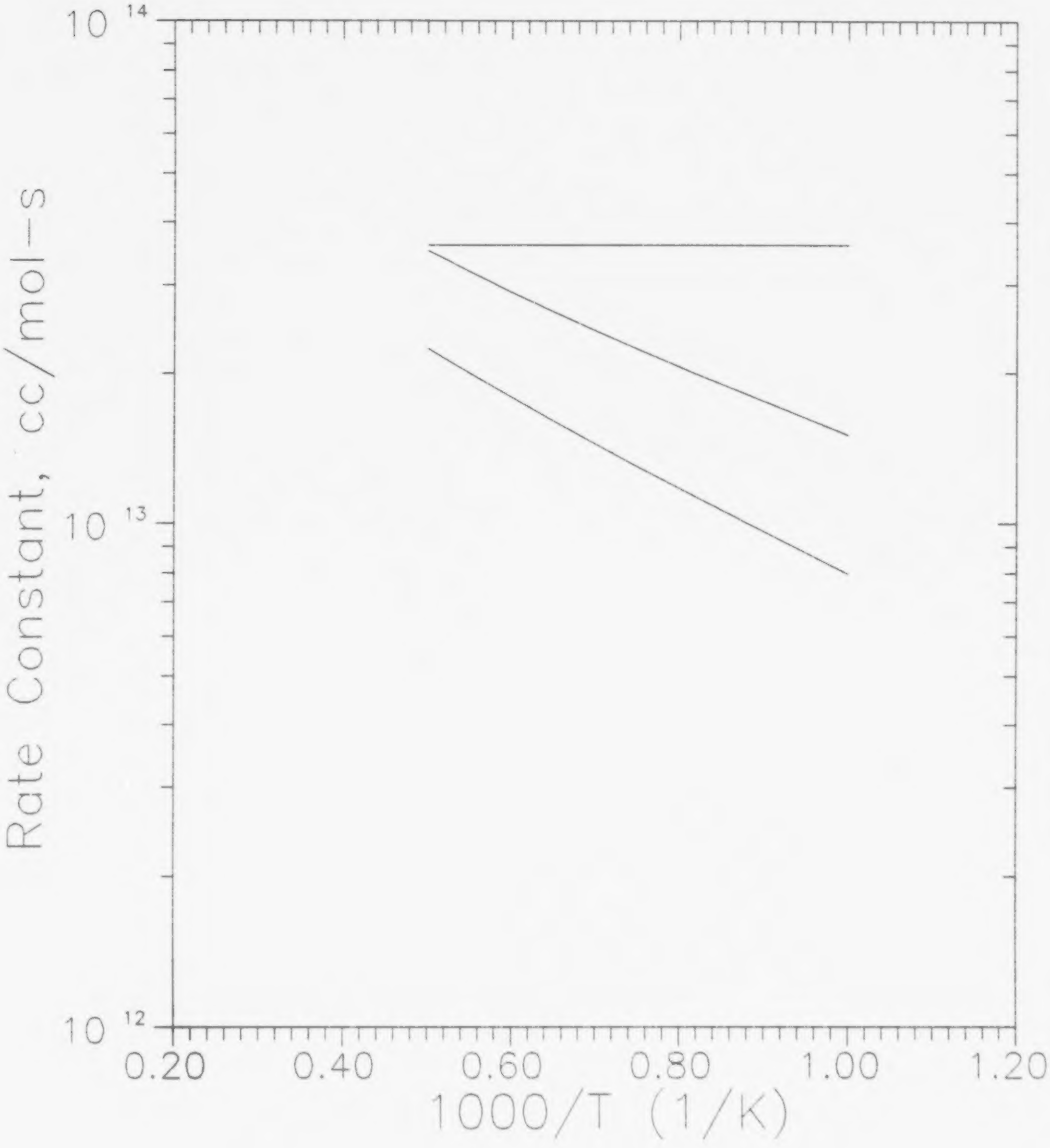
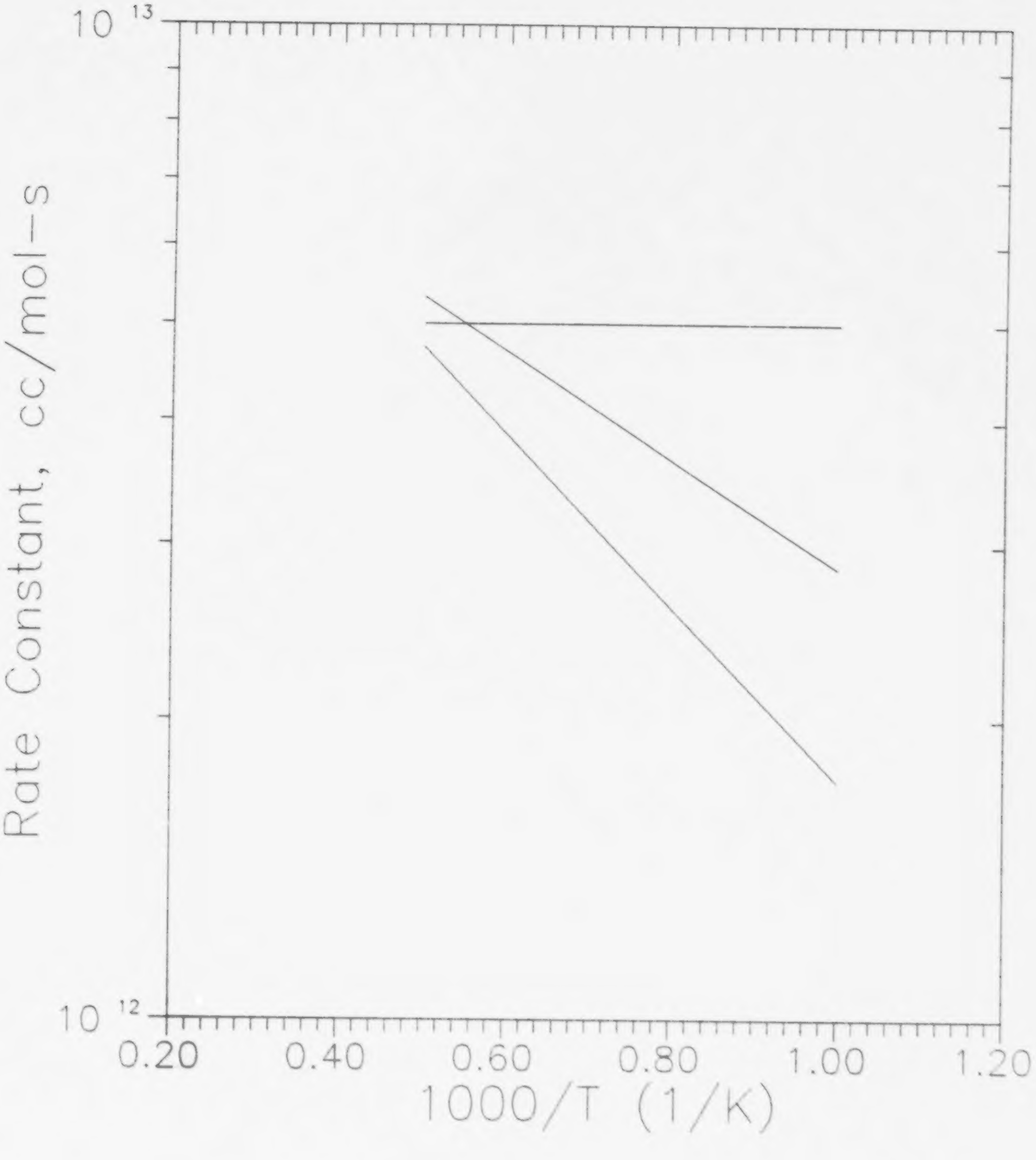
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HNO + M = H + NO + M**


10 14
10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HNO + HO = NO + H2O**


10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HNO + H = H2 + NO**

```
*---------------------------------------------------------------------------*
! File: NCOMECH.DAT                                                         !
! Saved: 08-04-88 at 11:08:01 am                                            !
*                                                                  Page  1  !
*---------------------------------------------------------------------------*

 1C    + 1NO          = 1CN   + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                 5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986                 6.6E+13 0.000  0.000  1000.0  2000.0

 1C    + 1N2O         = 1CN   + 1NO
Forward Rate Parameters:
Glarborg, et al. 1985
Glarborg, et al. 1986                 1.0E+13 0.000  0.000  1000.0  2000.0

 1CN   + 1O           = 1CO   + 1N
Forward Rate Parameters:
Glarborg, et al. 1985
Glarborg, et al. 1986                 1.8E+13 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985
                                      6.3E+11 0.500  0.000  1000.0  2000.0

 1CN   + 1O2          = 1NCO  + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                 5.6E+12 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                   3.2E+12 0.000  1.000  1000.0  2000.0

 1CN   + 1CO2         = 1NCO  + 1CO
Forward Rate Parameters:
Seeker, et al. 1985
                                      4.0E+11 0.500  7.000  1000.0  2000.0

 1CN   + 1NO2         = 1NCO  + 1NO
Forward Rate Parameters:
Glarborg, et al. 1985
Glarborg, et al. 1986                 3.0E+13 0.000  0.000  1000.0  2000.0

 1CN   + 1N2O         = 1NCO  + 1N2
Forward Rate Parameters:
Glarborg, et al. 1985
Glarborg, et al. 1986                 1.0E+13 0.000  0.000  1000.0  2000.0

 1C2N2 + 1O           = 1NCO  + 1CN
Forward Rate Parameters:
Glarborg, et al. 1985
Glarborg, et al. 1986                 4.6E+12 0.000  8.880  1000.0  2000.0

 1NCO  + 1O           = 1NO   + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985                 3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986                 5.6E+13 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985                   5.0E+11 0.500  6.875  1000.0  2000.0

 1NCO  + 1N           = 1N2   + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985
Glarborg, et al. 1985                 2.0E+13 0.000  0.000  1000.0  2000.0

 1NCO  + 1M           = 1N    + 1CO   + 1M
Forward Rate Parameters:
Glarborg, et al. 1985                 3.1E+16-0.500 48.000  1000.0  2000.0
```

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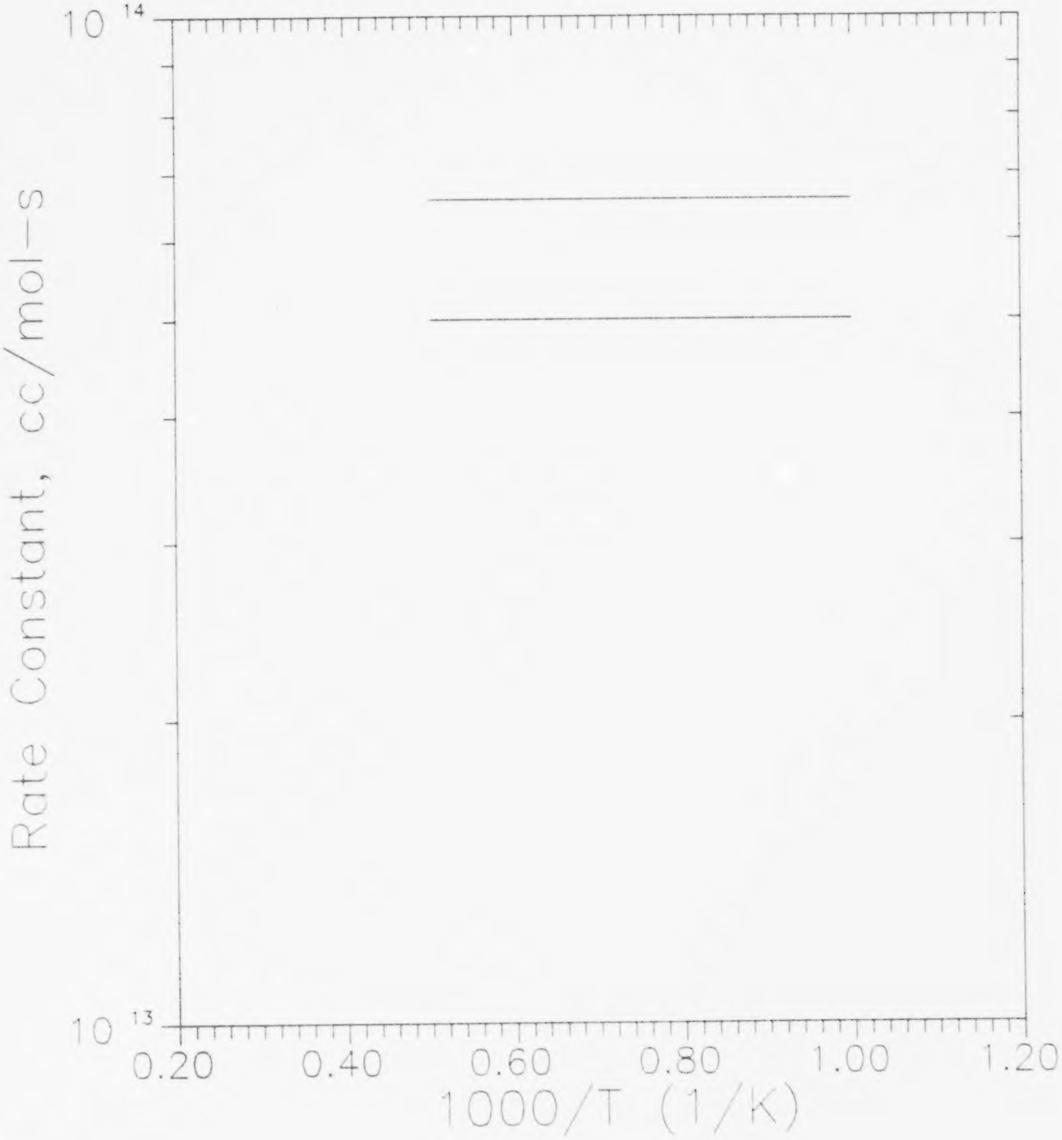
*-----------------------------------------------------------------------*
| File: NCOMECH.DAT                                                     |
| Saved: 08-04-88 at 11:08:01 am                                        |
|                                                              Page  2  |
*-----------------------------------------------------------------------*

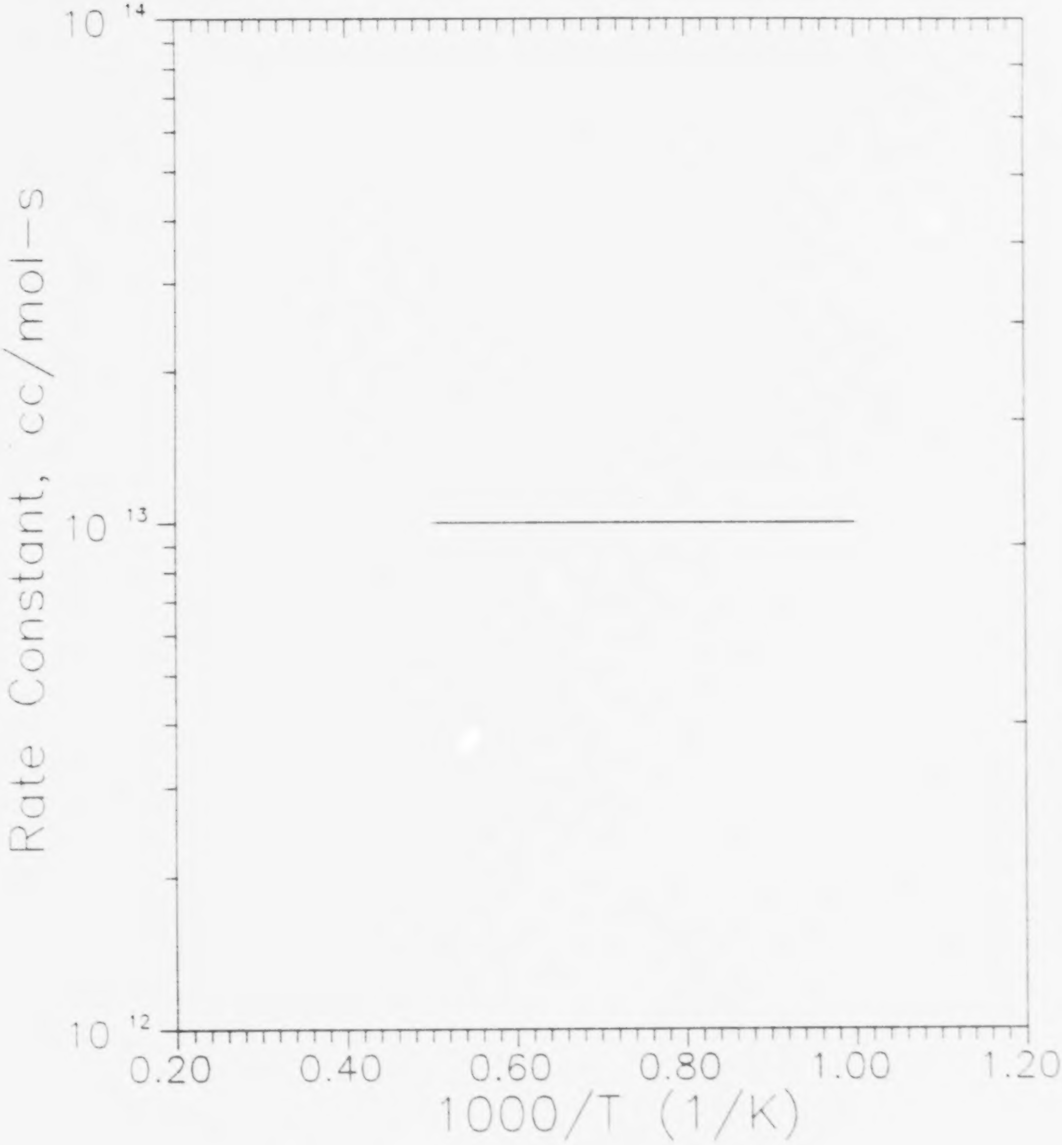
Glarborg, et al. 1986

 1NCO  + 1NO          = 1N2O  + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985                     1.0E+13 0.000 -0.390  1000.0  2000.0
Glarborg, et al. 1986

 1N    + 1CO2         = 1NO   + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985                     1.9E+11 0.000  3.400  1000.0  2000.0
Glarborg, et al. 1986
```

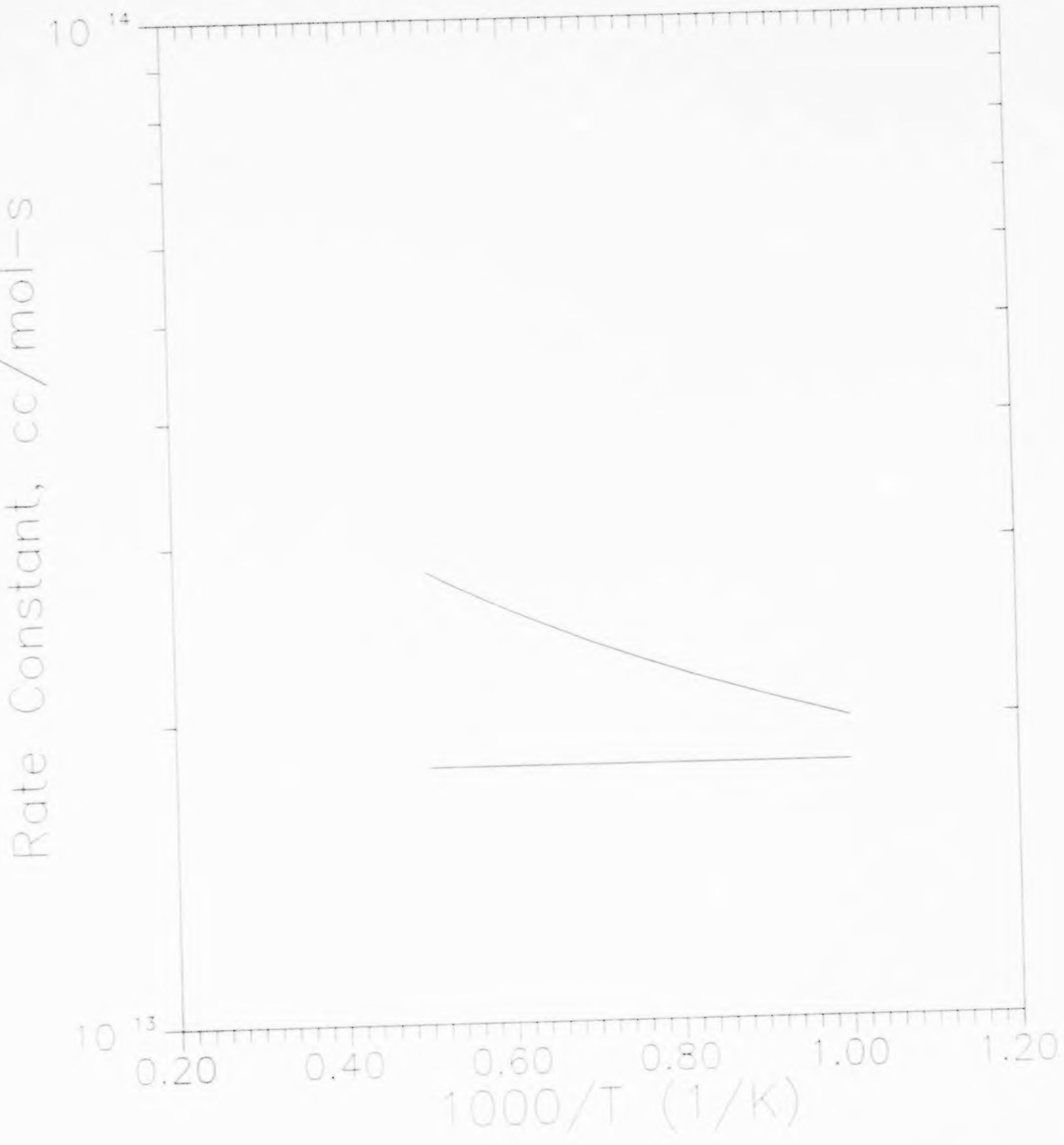

10 ¹⁴
10 ¹³
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**C + NO = CN + O**



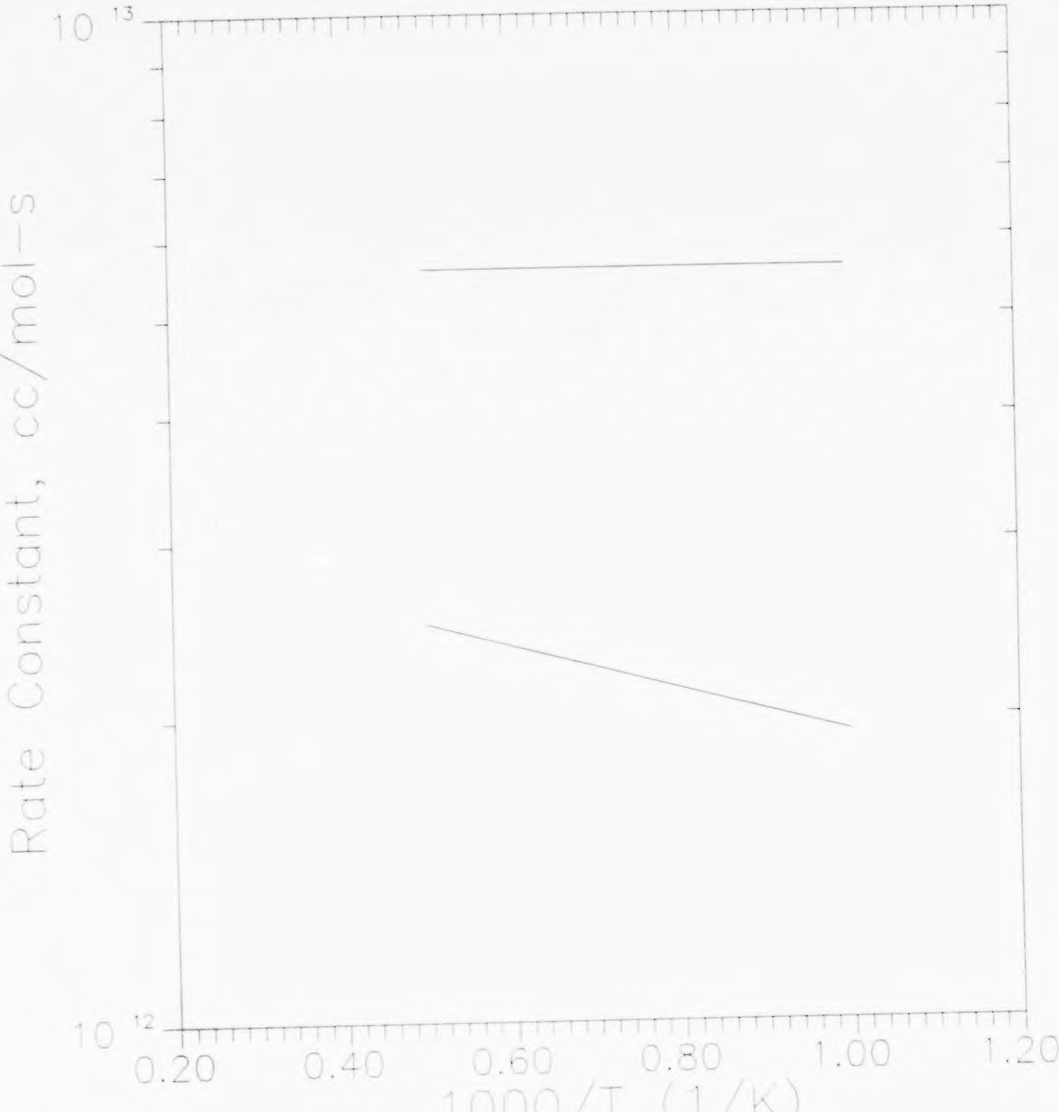
Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**C + N2O = CN + NO**



10^14
10^13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CN + O = CO + N**


10 13
10 12
Rate Constant, cc/mol-s
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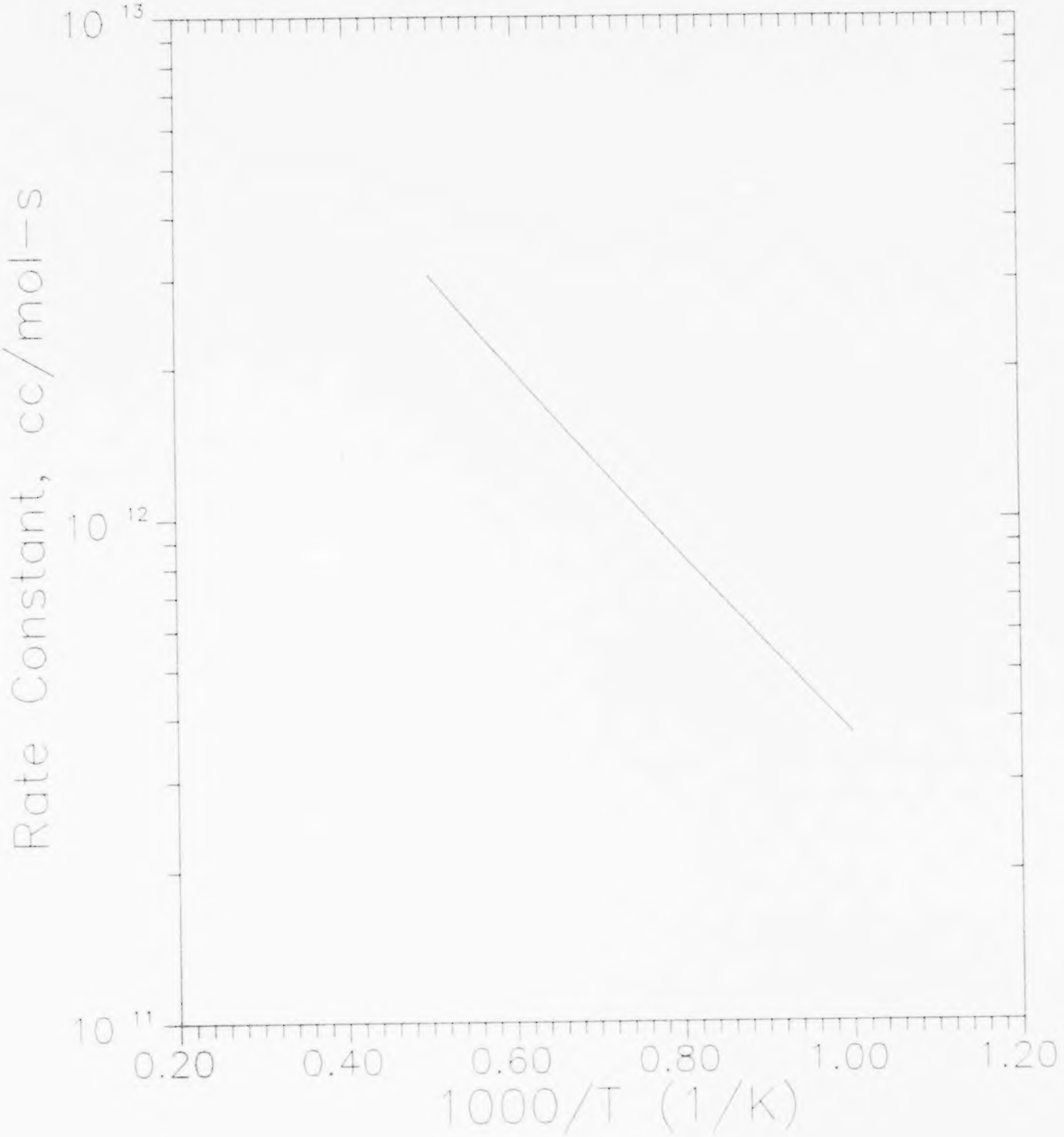
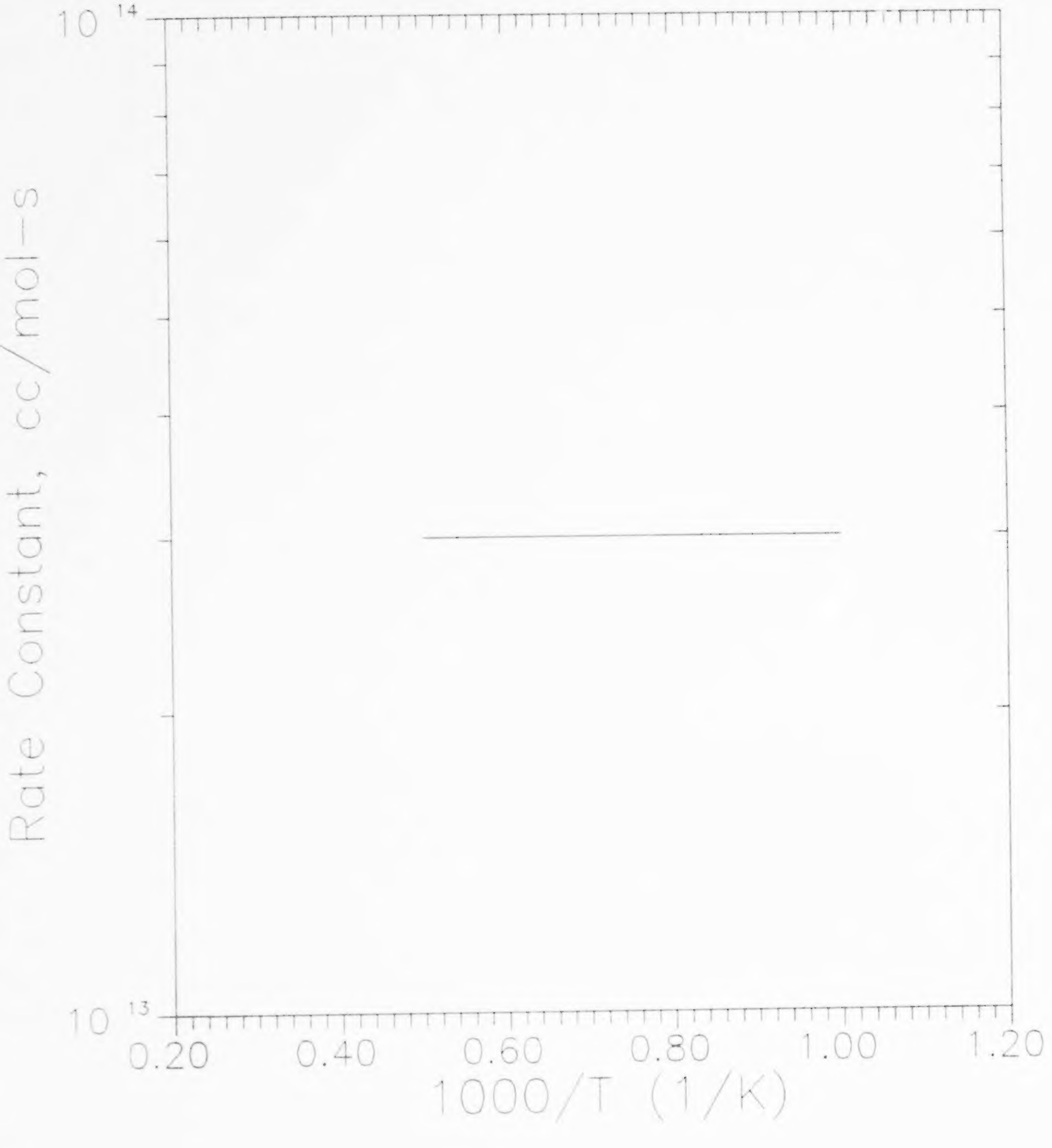
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CN + O2 = NCO + O**

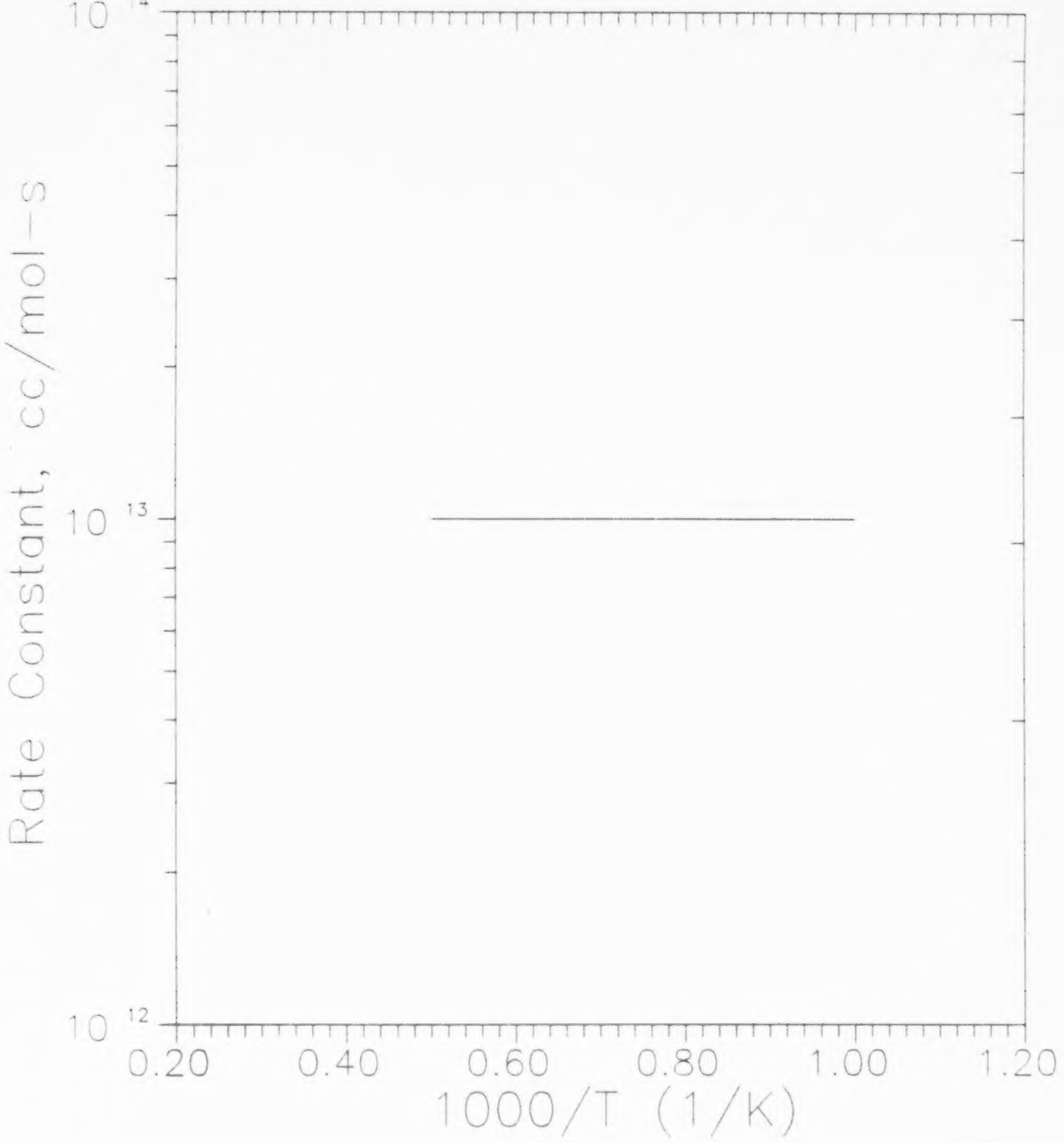


Rate Constant, cc/mol-s
10^13
10^12
10^11
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

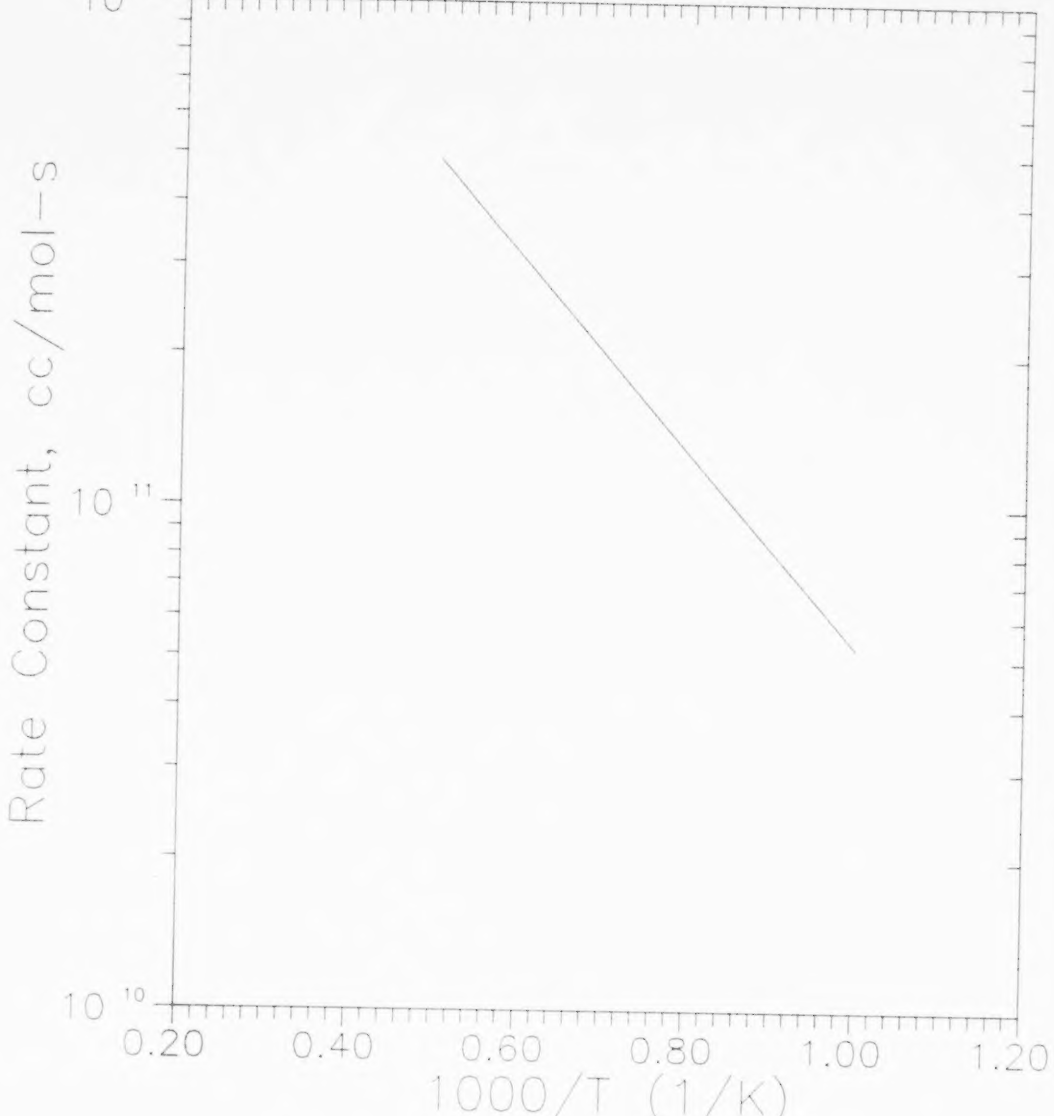
**CN + CO2 = NCO + CO**


10 ^14
10 ^13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

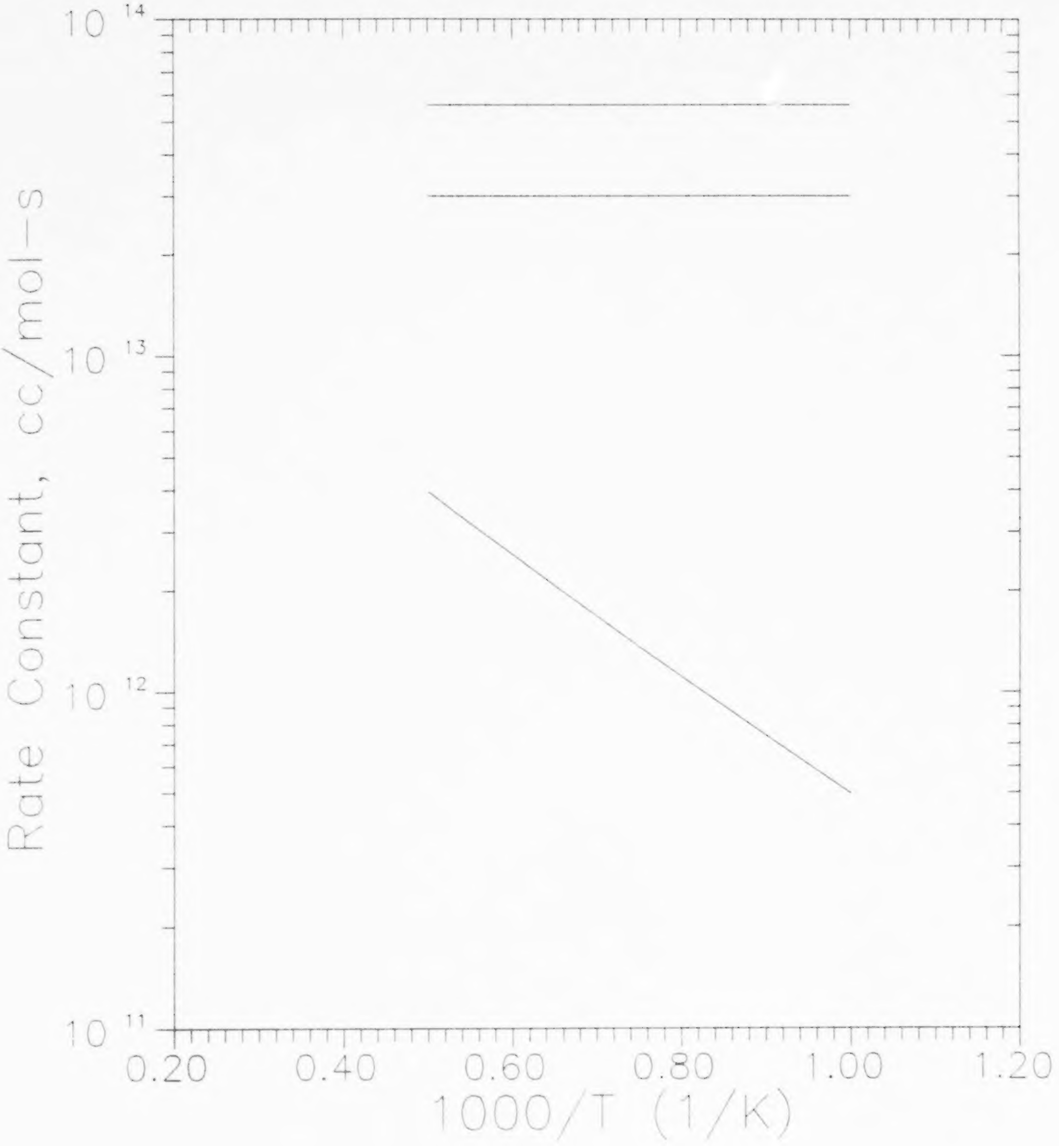
**CN + NO2 = NCO + NO**


10^14
10^13
10^12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CN + N2O = NCO + N2**

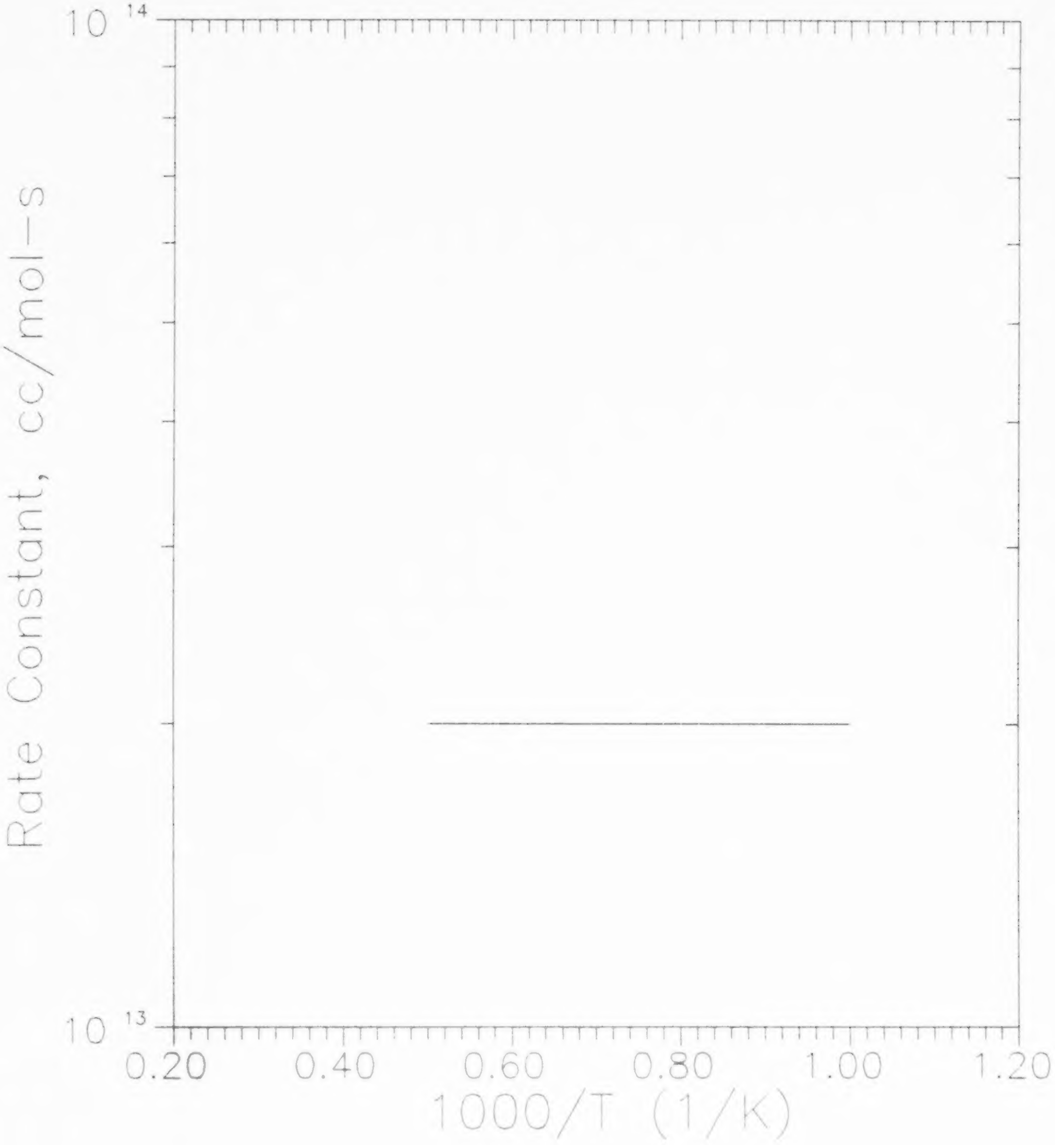

10 12
10 11
10 10
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**C2N2 + O = NCO + CN**

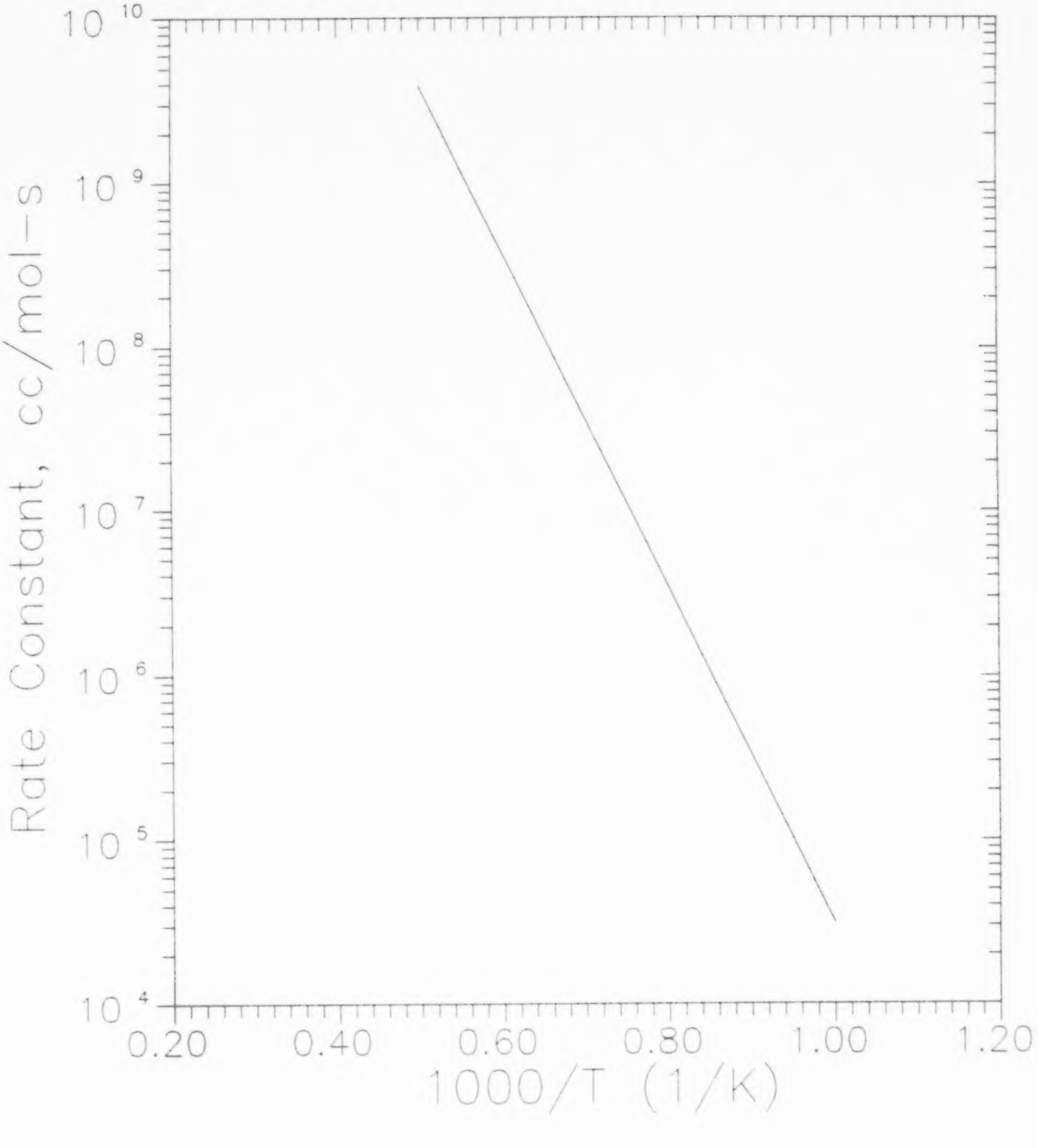


$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

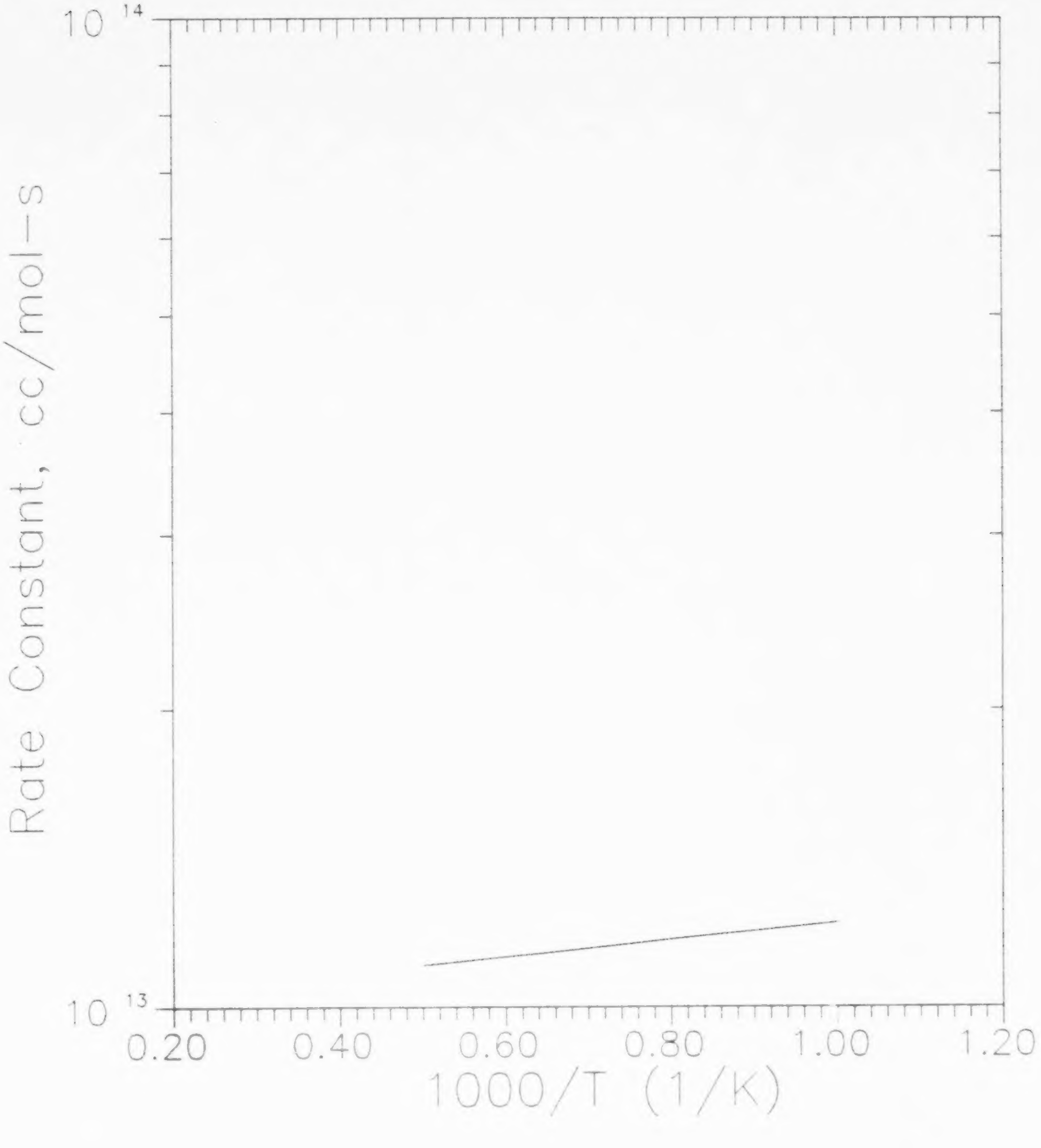
**NCO + O = NO + CO**


10 14
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

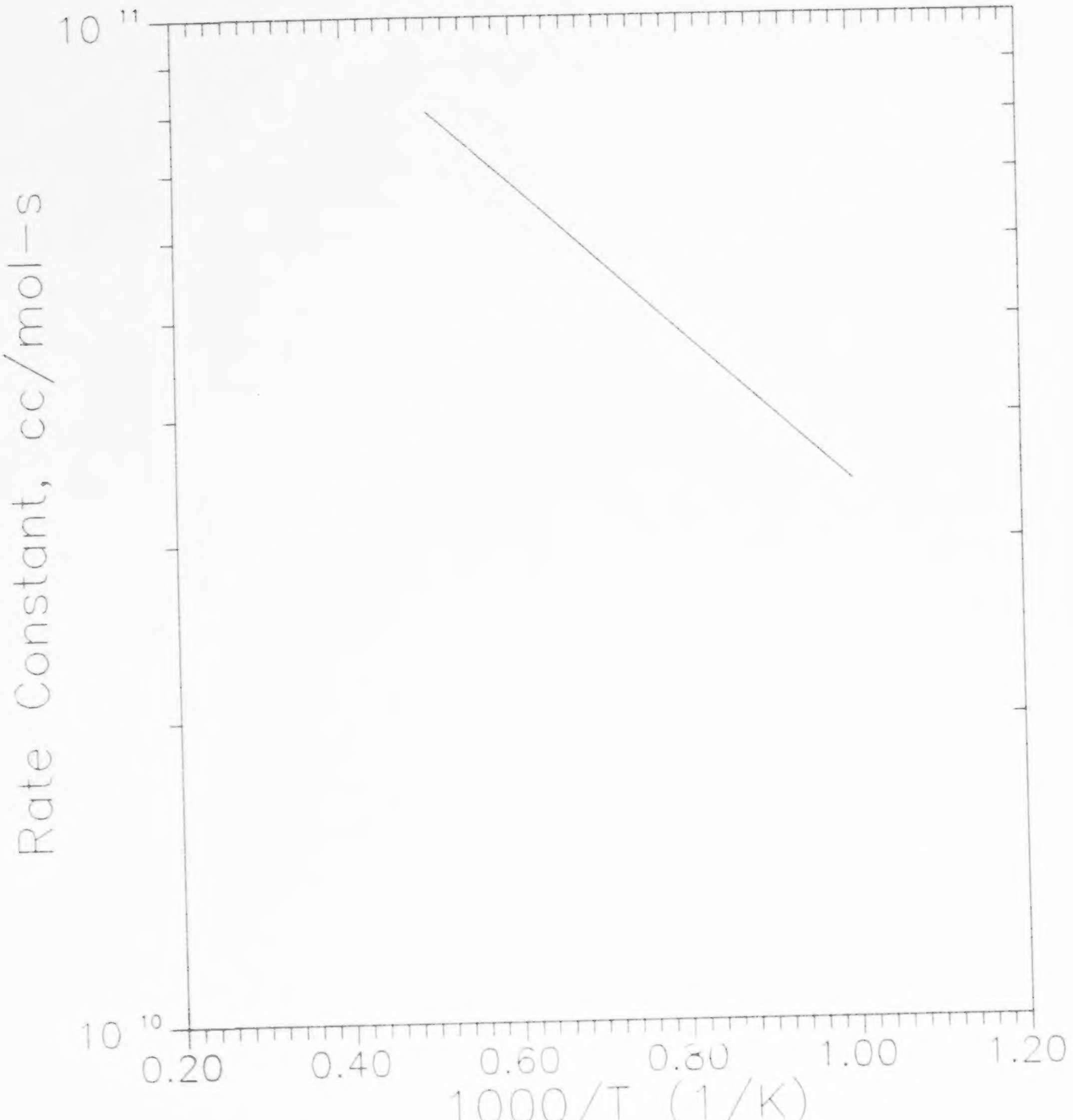
**NCO + N = N2 + CO**


Rate Constant, cc/mol-s
$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
$10^{5}$
$10^{4}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NCO + M = N + CO + M**


10 $^{14}$
Rate Constant, cc/mol-s
10 $^{13}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NCO + NO = N2O + CO**



10^11
10^10
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**N + CO2 = NO + CO**

```
*-----------------------------------------------------------------------*
|  File: HCNMECH.DAT                                                    |
|  Saved: 08-04-88 at 11:07:19 am                              Page  1  |
*-----------------------------------------------------------------------*

 1CH4  + 1N            = 1NH   + 1CH3
Forward Rate Parameters:
Glarborg, et al. 1985                   1.0E+13 0.000 24.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH4  + 1CN           = 1CH3  + 1CHN
Forward Rate Parameters:
Glarborg, et al. 1986                   3.2E+11 0.700  5.000  1000.0  2000.0

 1CH3  + 1N            = 1CHN  + 1H    + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH3  + 1CN           = 1CH2  + 1CHN
Forward Rate Parameters:
Glarborg, et al. 1986                   1.0E+11 0.700  3.000  1000.0  2000.0

 1CH2  + 1N2           = 1CHN  + 1NH
Forward Rate Parameters:

Glarborg, et al. 1985                   1.0E+14 0.000 60.000  1000.0  2000.0
Seeker, et al. 1985
Glarborg, et al. 1986                   1.0E+13 0.000 74.000  1000.0  2000.0

 1CH2  + 1NH           = 1CHN  + 1H    + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH2  + 1N            = 1CHN  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH   + 1N2           = 1CHN  + 1N
Forward Rate Parameters:
Glarborg, et al. 1985                   1.0E+11 0.000 13.600  1000.0  2000.0
Glarborg, et al. 1986                   1.9E+11 0.000 13.600  1000.0  2000.0
This work                               1.49E12 0.000 13.600  1000.0  2000.0
Reverse Rate Parameters:
Seeker, et al. 1985                     2.5E+11 0.000 16.000  1000.0  2000.0

 1CH   + 1N            = 1CN   + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986                   1.3E+13 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985                     6.3E+11 0.500  0.000  1000.0  2000.0

 1CH   + 1NH2          = 1CHN  + 1H    + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                   3.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CH   + 1NH           = 1CHN  + 1H
```

```
*-----------------------------------------------------------------------------*
|  File: HCNMECH.DAT                                                          |
| Saved: 08-04-88 at 11:07:19 am                                    Page  2 |
*-----------------------------------------------------------------------------*

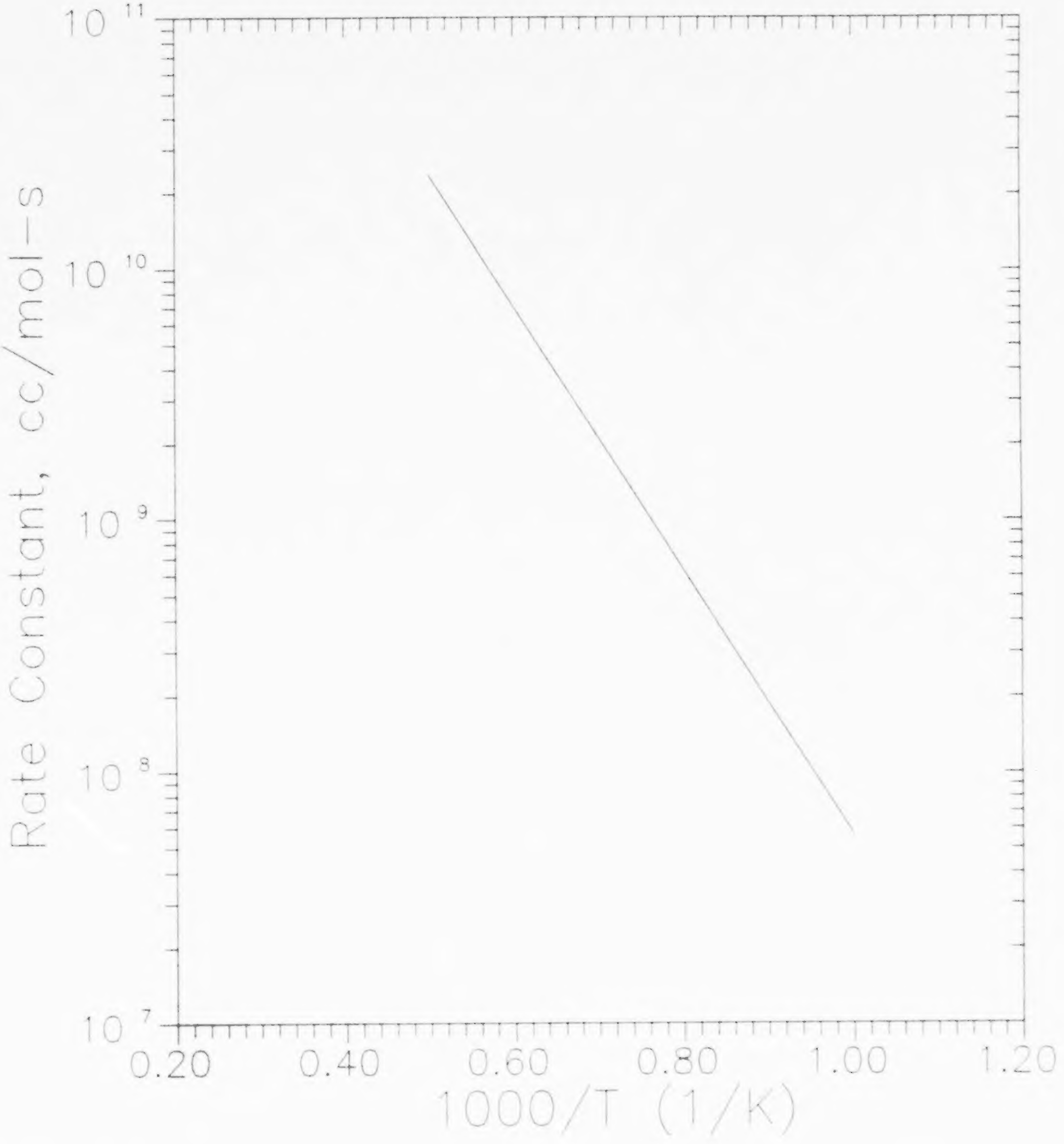
Forward Rate Parameters:
Glarborg, et al. 1985
Glarborg, et al. 1986                  5.0E+13 0.000  0.000  1000.0  2000.0

 1CHN  + 1CN         = 1C2N2 + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                  2.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1CN   + 1H2         = 1CHN  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                  5.5E+11 0.700  4.890  1000.0  2000.0
Glarborg, et al. 1986                  3.0E+05 2.450  2.237  1000.0  2000.0
Seeker, et al. 1985                    6.2E+12 0.000  5.300  1000.0  2000.0

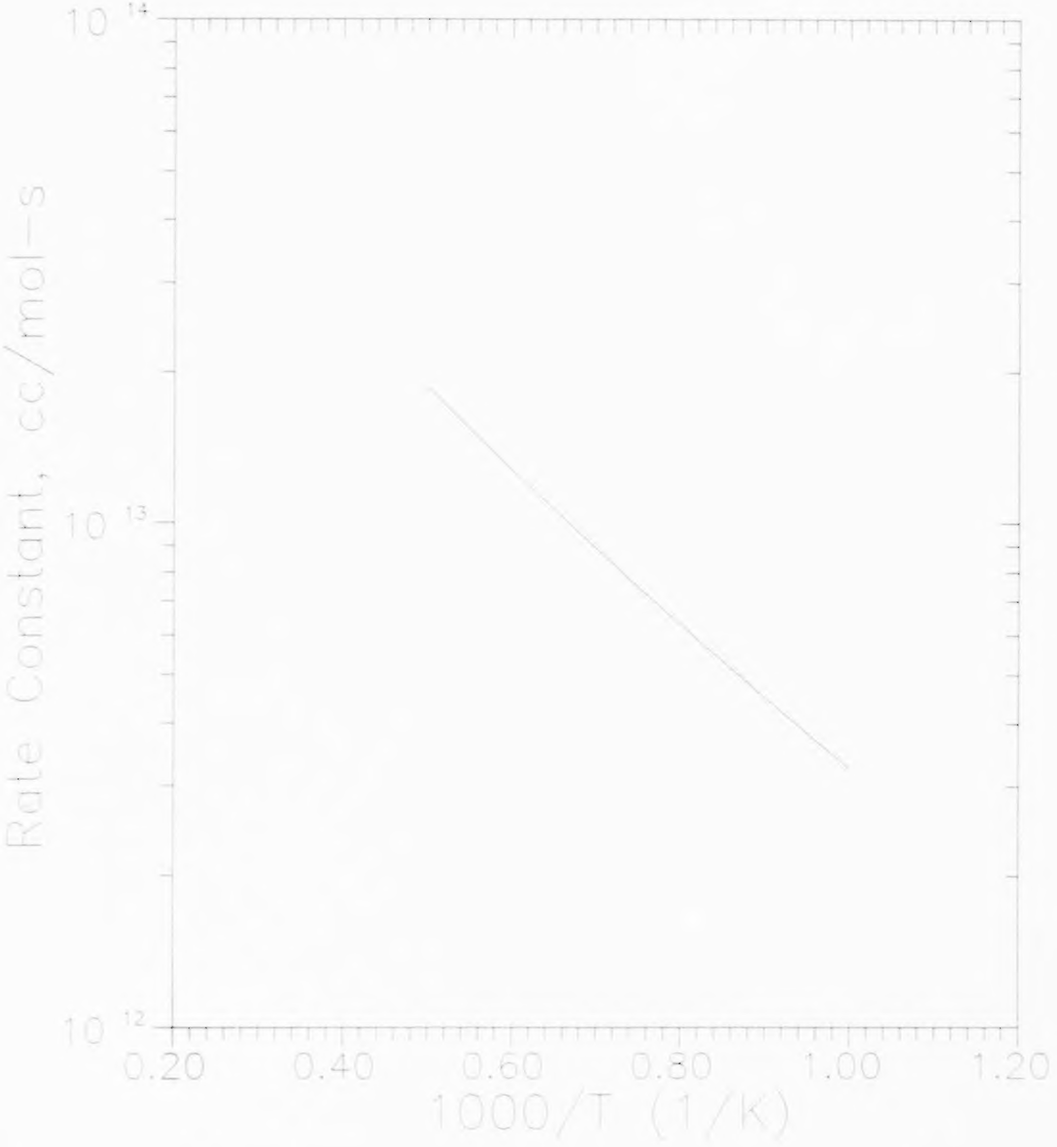
 1CN   + 1NH3        = 1CHN  + 1NH2
Forward Rate Parameters:
Seeker, et al. 1985                    7.0E+10 0.700  2.000  1000.0  2000.0

 1CN   + 1NH2        = 1CHN  + 1NH
Forward Rate Parameters:
Seeker, et al. 1985                    5.0E+10 0.700  2.000  1000.0  2000.0
```

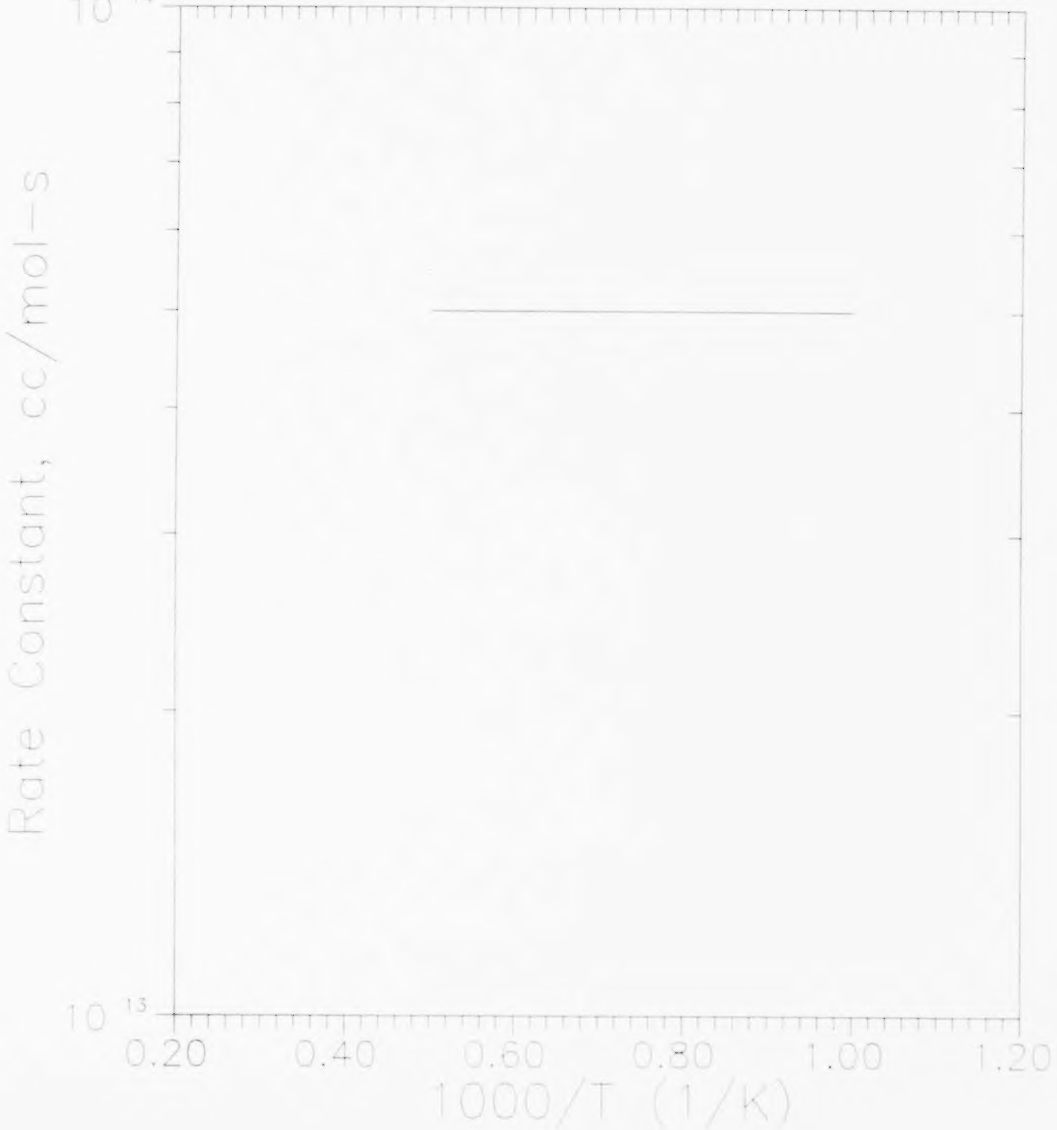


10 11
10 10
10 9
10 8
10 7
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

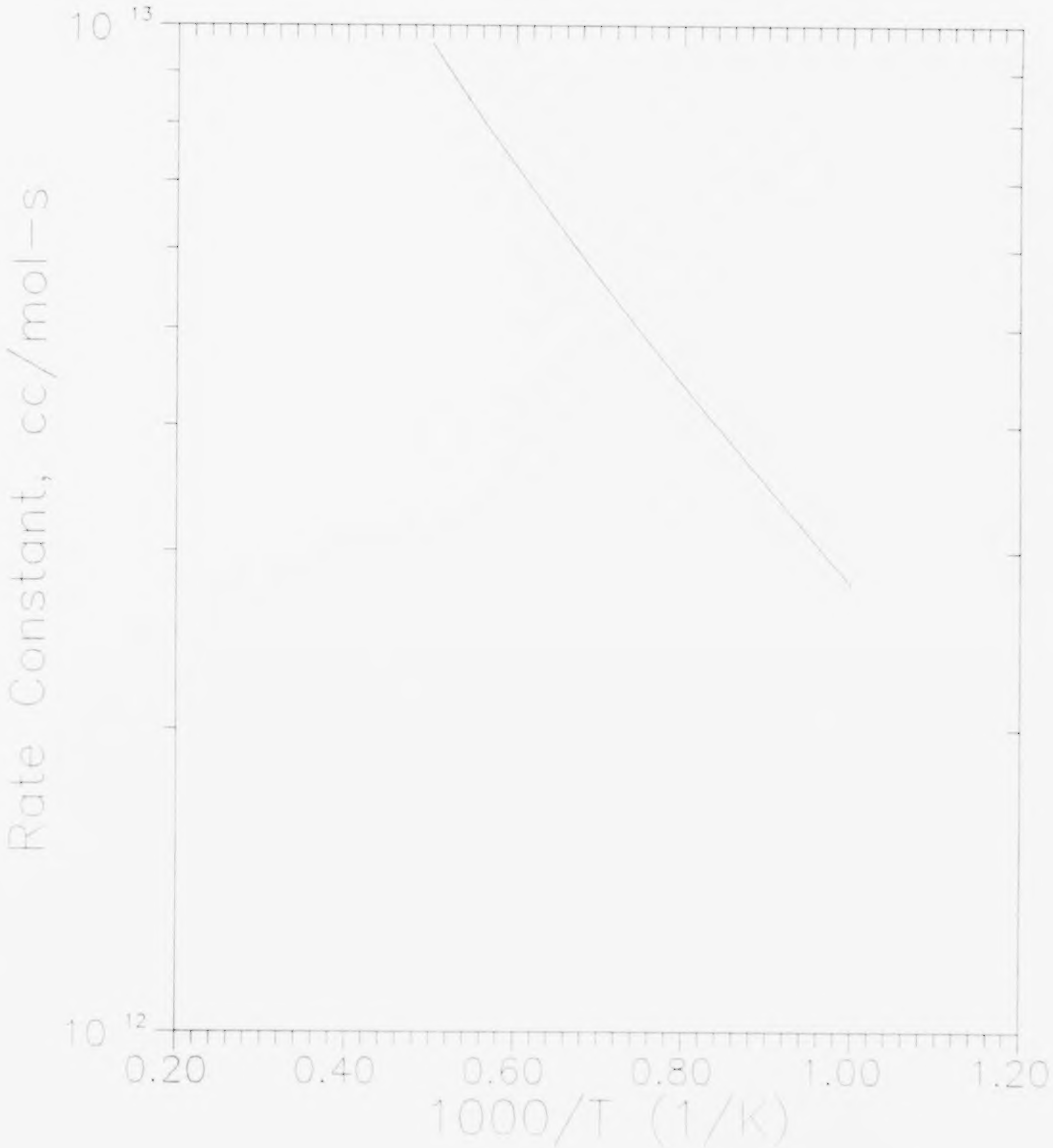
**CH4 + N = NH + CH3**



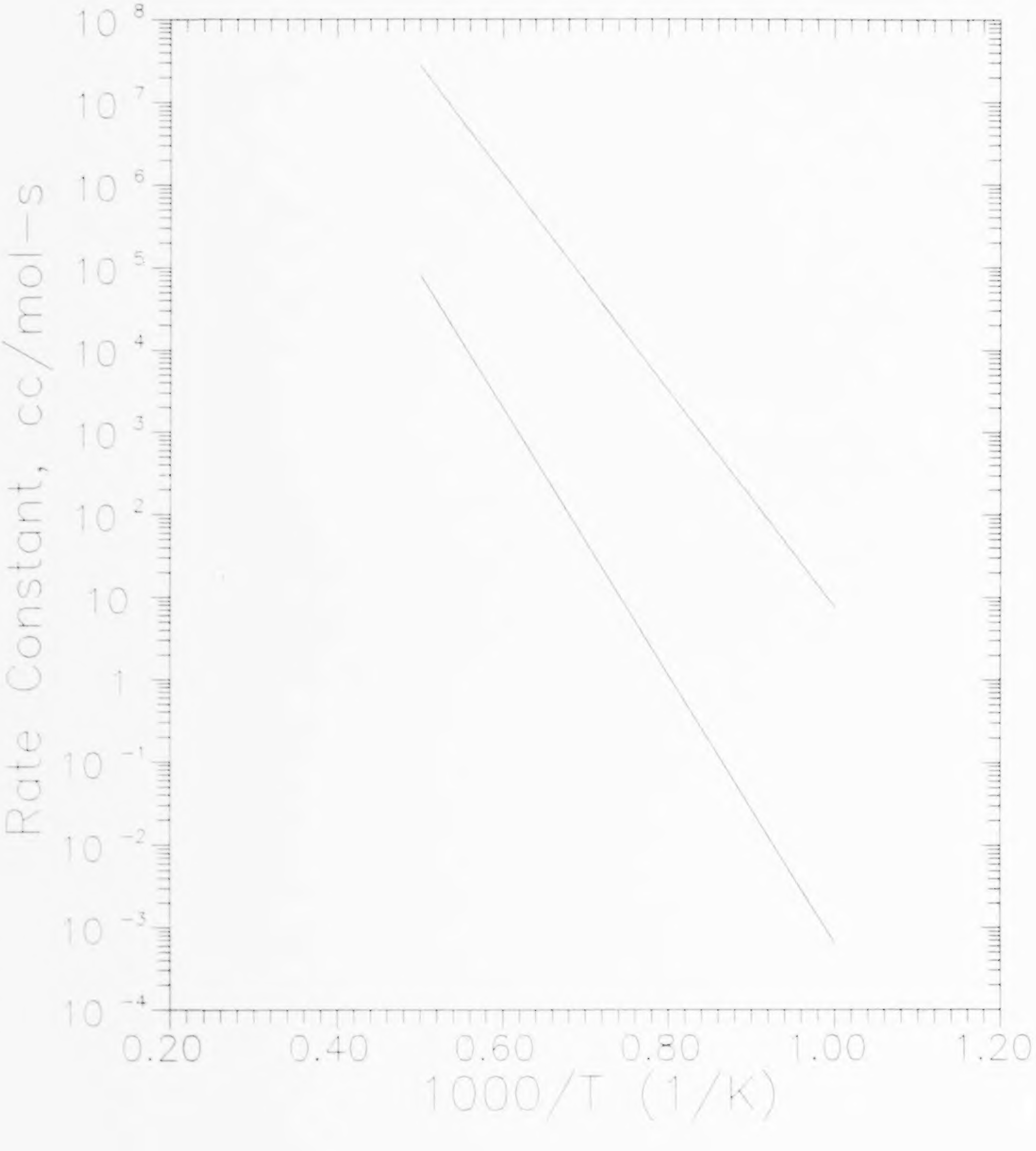
**$CH_4$ + CN = $CH_3$ + CHN**


10 14
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH3 + N = CHN + H + H**

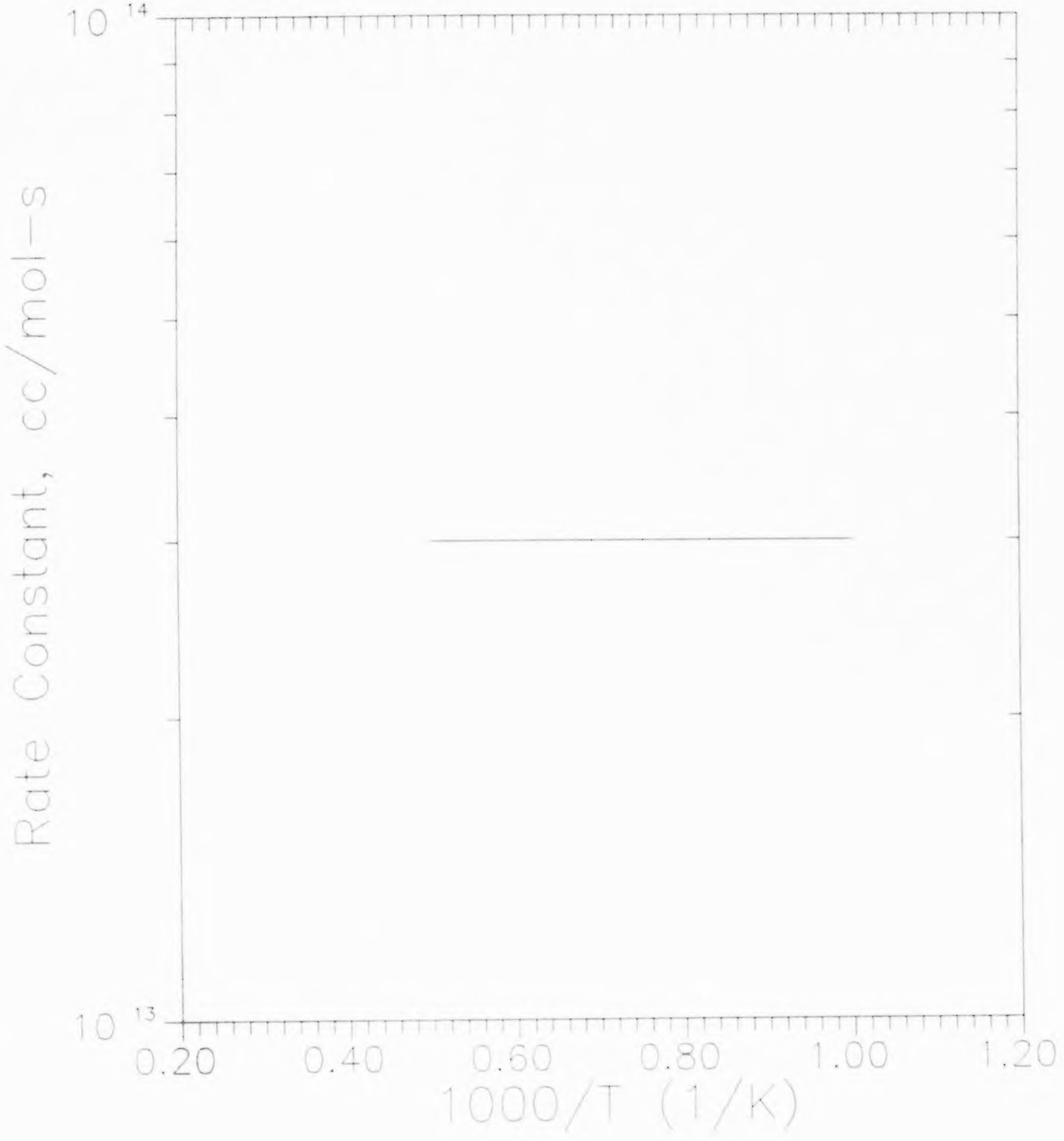


**CH3 + CN = CH2 + CHN**

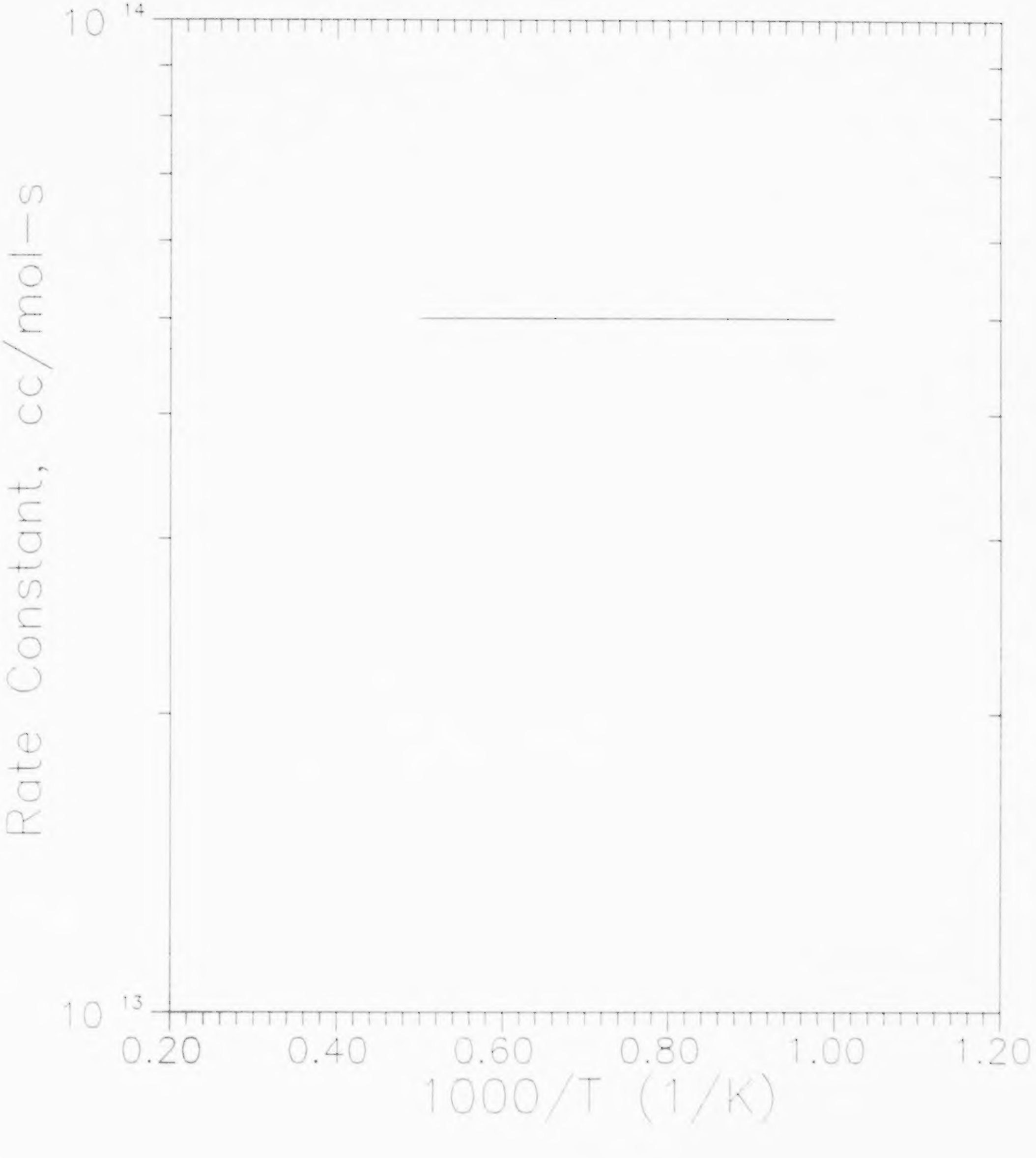


Rate Constant, cc/mol-s
$10^8$
$10^7$
$10^6$
$10^5$
$10^4$
$10^3$
$10^2$
10
1
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

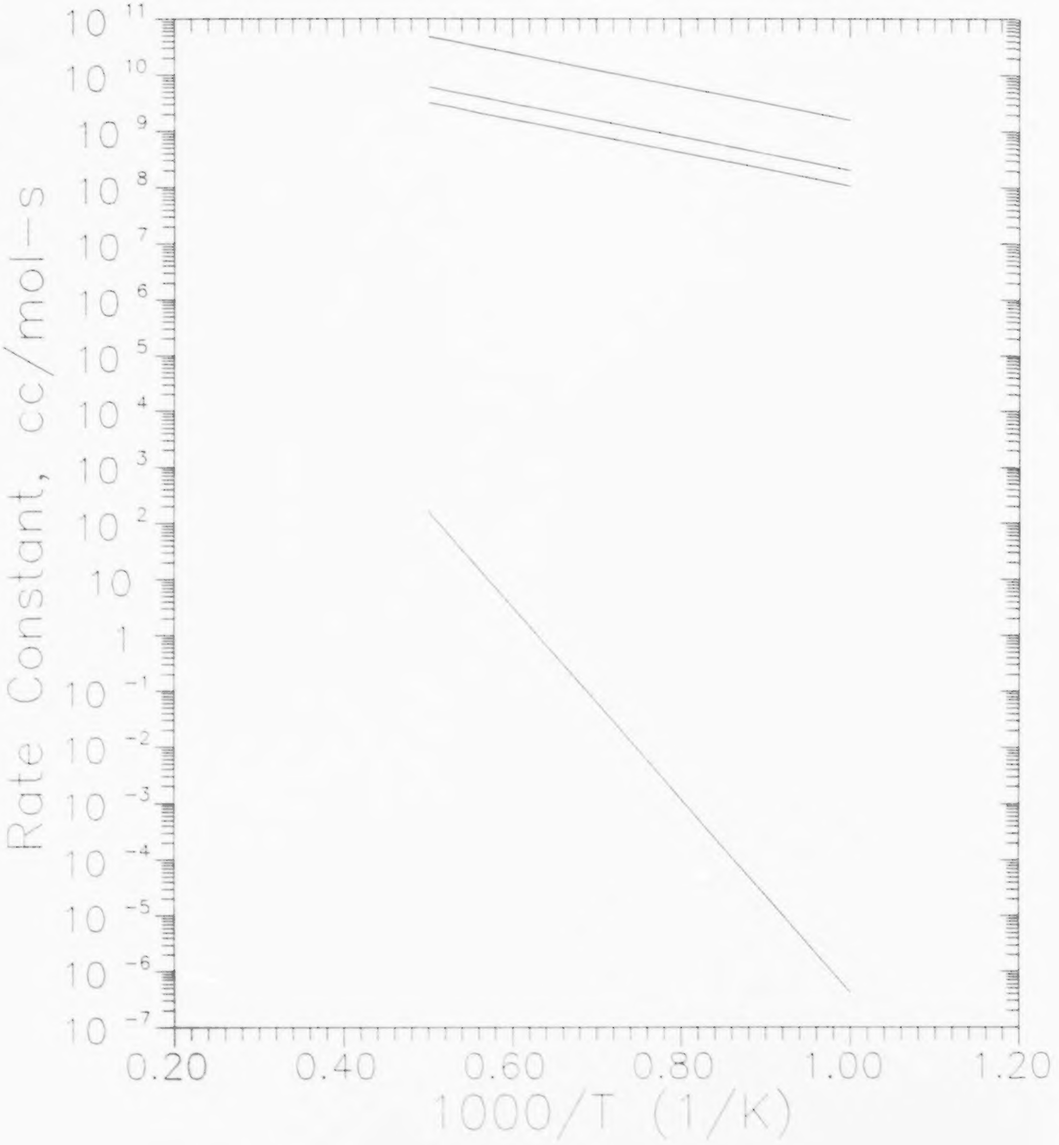
**CH2 + N2 = CHN + NH**


10 14
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + NH = CHN + H + H**

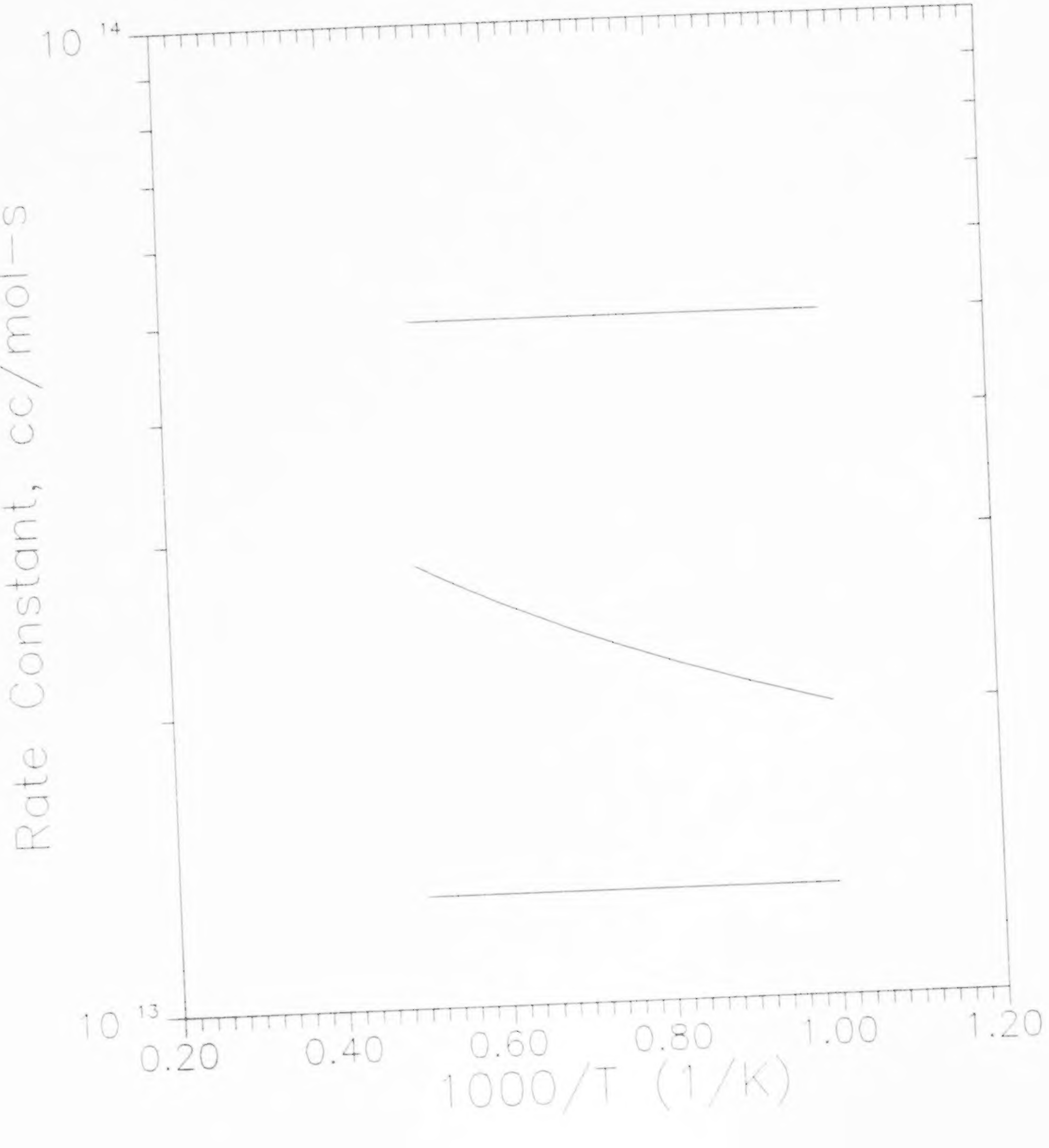

Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + N = CHN + H**

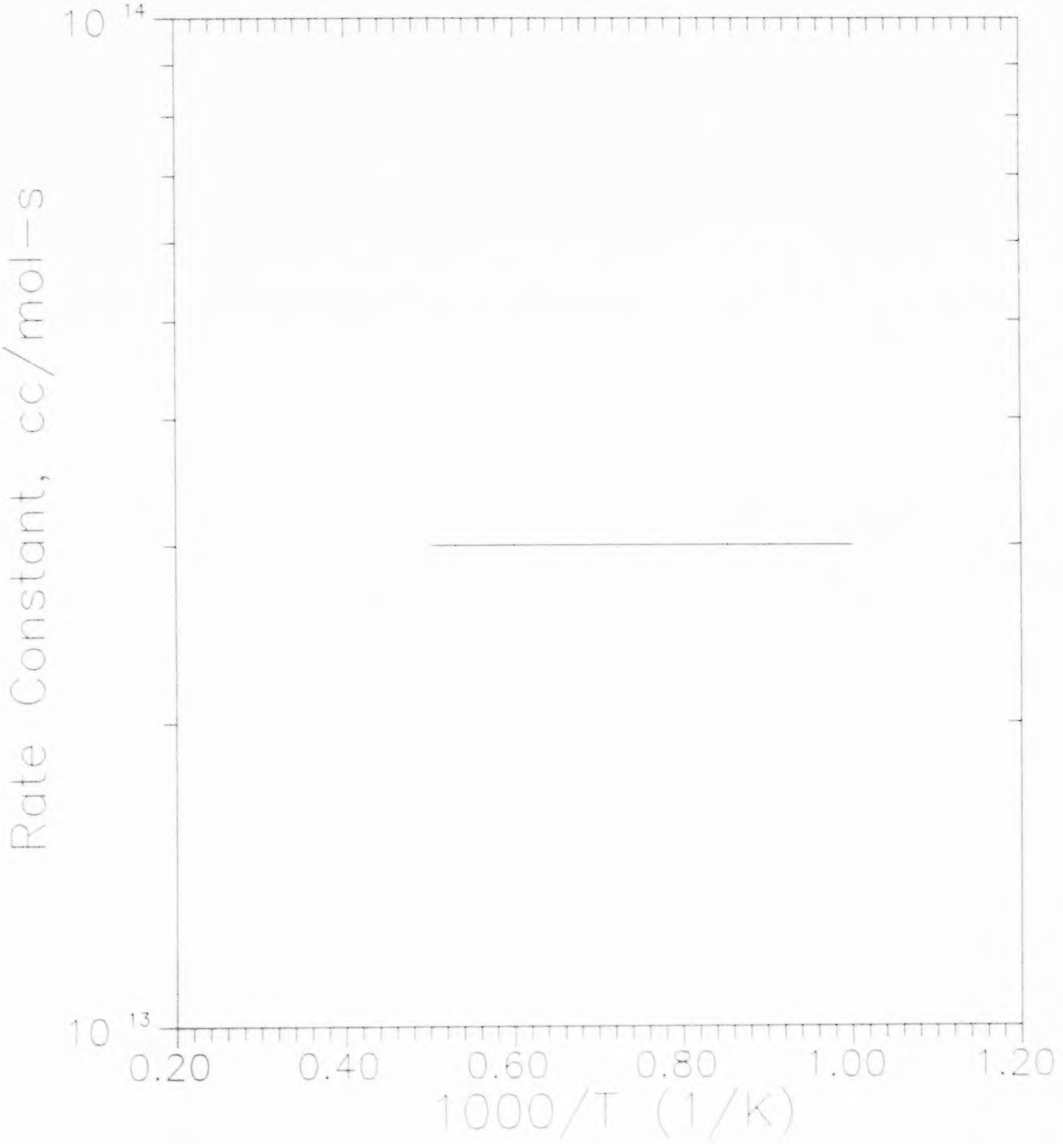


Rate Constant, cc/mol-s
$10^{11}$
$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
$10^{5}$
$10^{4}$
$10^{3}$
$10^{2}$
10
1
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
$10^{-5}$
$10^{-6}$
$10^{-7}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

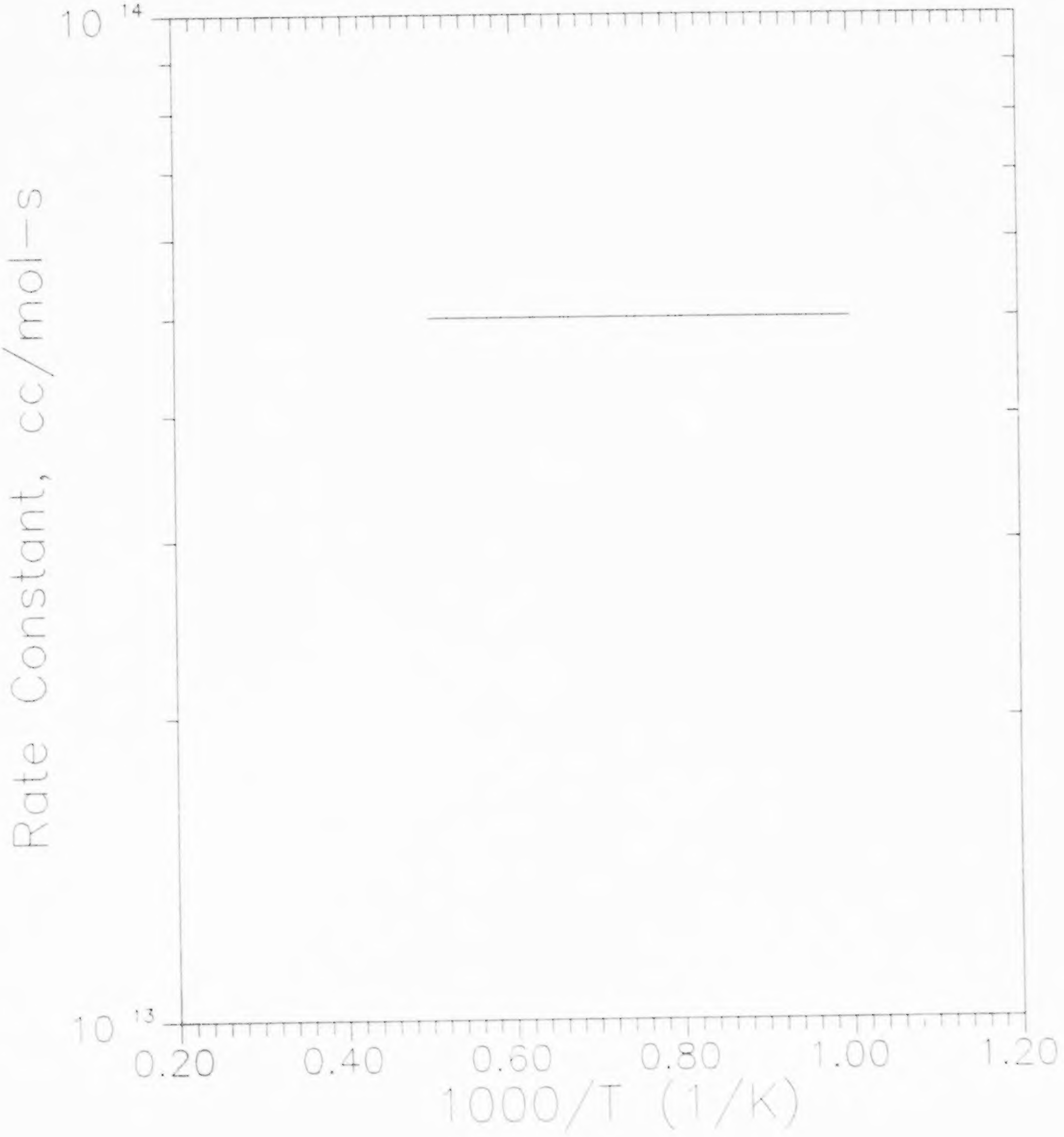
**CH + N2 = CHN + N**


10 14
10 13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

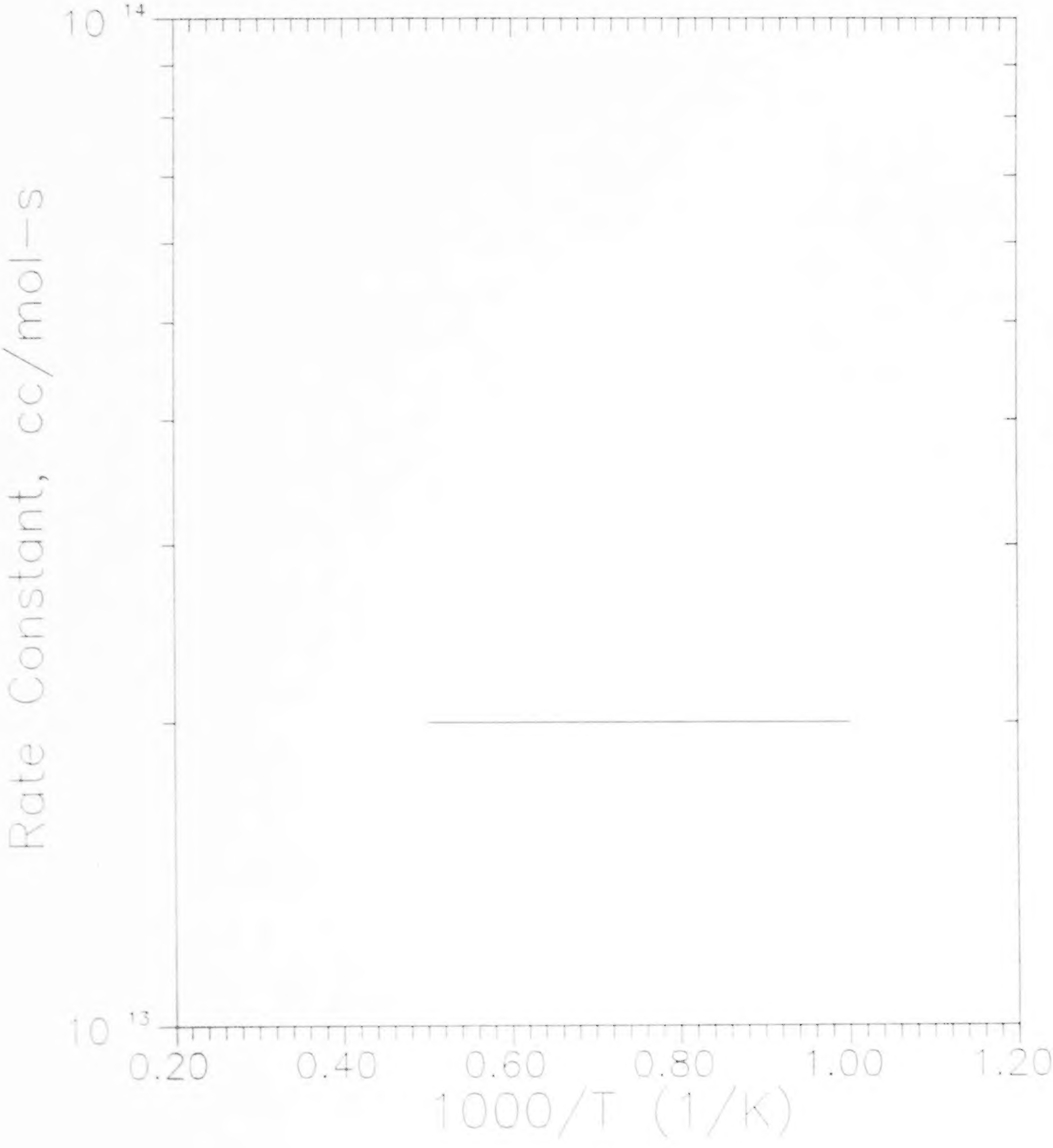
CH + N = CN + H


10^14
10^13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

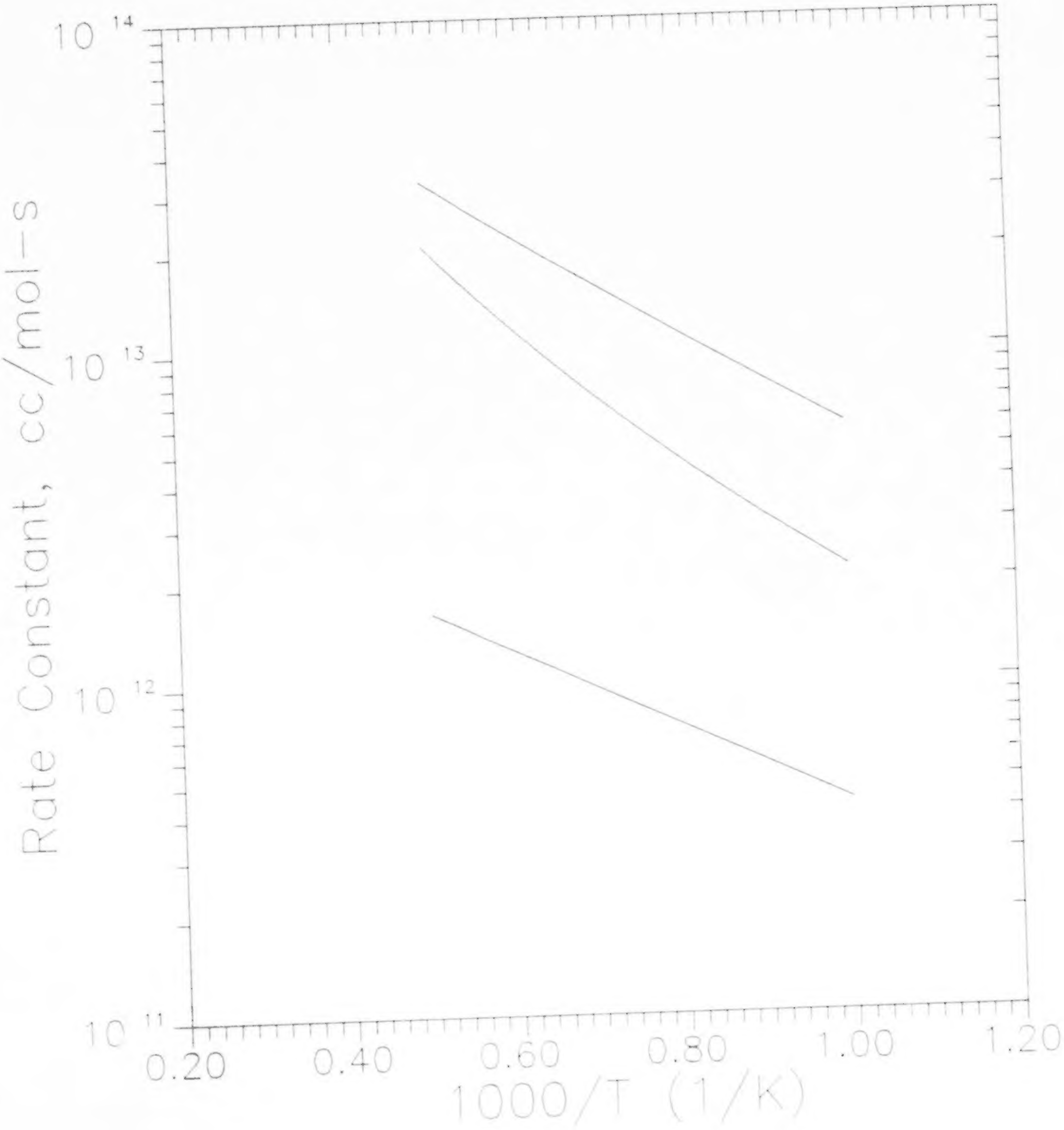
CH + NH2 = CHN + H + H


$10^{14}$
$10^{13}$
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH + NH = CHN + H**


10^14
10^13
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CHN + CN = C2N2 + H**


$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
Rate Constant, cc/mol-s
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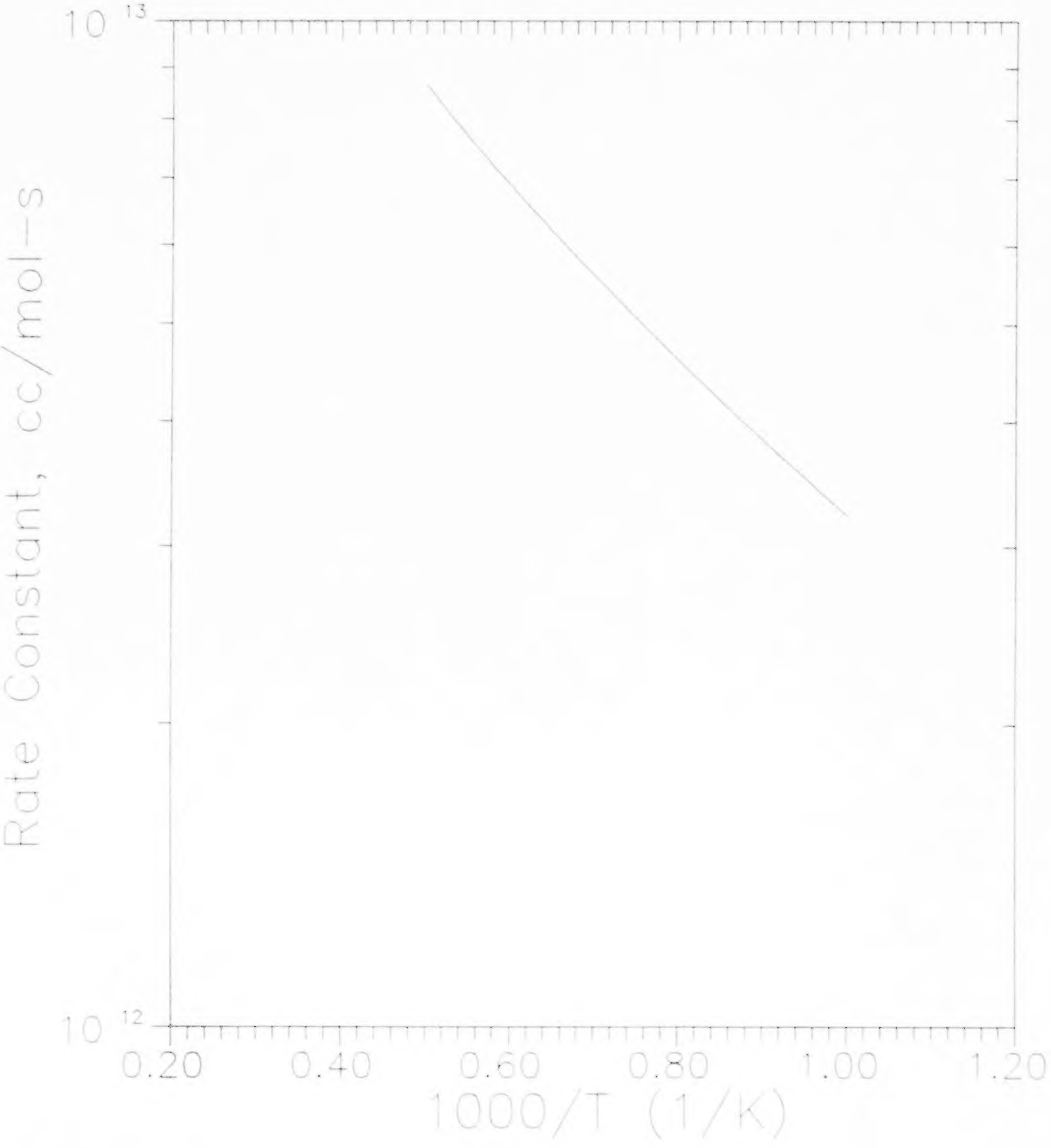
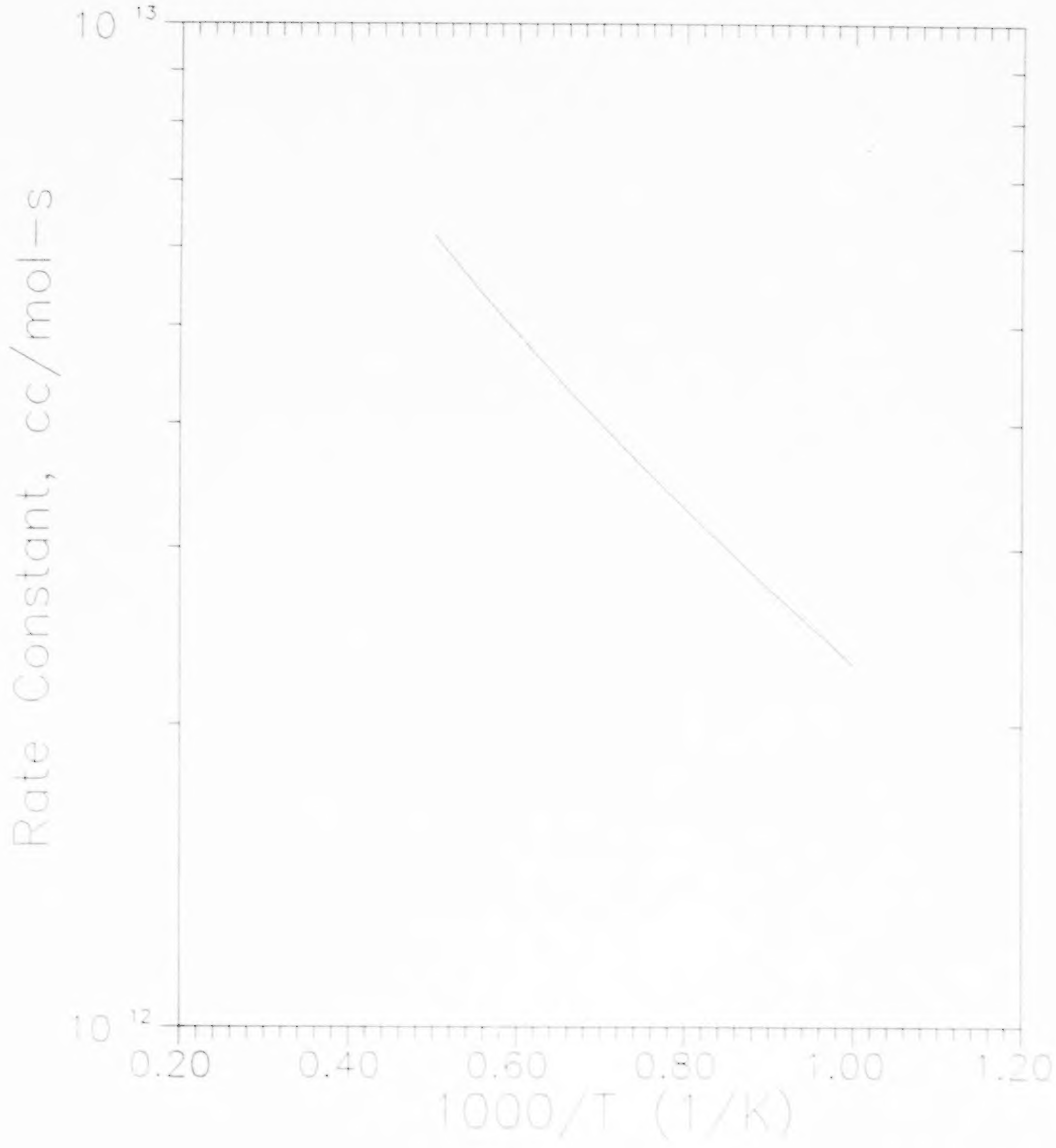
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CN + H2 = CHN + H**



**CN + NH3 = CHN + NH2**



10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

CN + NH2 = CHN + NH

```
*---------------------------------------------------------------------------*
|  File: HNCOMECH.DAT                                                       |
| Saved: 08-04-88 at 11:18:15 am                                   Page  1 |
*---------------------------------------------------------------------------*

 1CHN  + 1HO           = 1CN   + 1H2O
Forward Rate Parameters:
Glarborg, et al. 1985                      4.4E+12 0.000  9.000  1000.0  2000.0
Glarborg, et al. 1986                      1.5E+13 0.000 10.900  1000.0  2000.0
Seeker, et al. 1985                        2.0E+11 0.500  5.000  1000.0  2000.0

 1CHN  + 1HO           = 1HOCN + 1H
Forward Rate Parameters:
Glarborg, et al. 1986                      9.2E+12 0.000 15.000  1000.0  2000.0
This work                                  4.6E+12 0.000 15.000  1000.0  2000.0

 1CHN  + 1HO           = 1HNCO + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                      4.8E+11 0.000 11.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                        2.0E+10 0.500  5.620  1000.0  2000.0

 1CHN  + 1O            = 1CN   + 1HO
Forward Rate Parameters:
Glarborg, et al. 1985                      2.7E+09 1.580 26.600  1000.0  2000.0
Glarborg, et al. 1986
Reverse Rate Parameters:
Seeker, et al. 1985                        3.2E+12 0.000  3.000  1000.0  2000.0

 1CHN  + 1O    + 1M    = 1CN   + 1HO   + 1M
Forward Rate Parameters:
Seeker, et al. 1985                        5.7E+16 0.000117.000  1000.0  2000.0

 1CHN  + 1O            = 1NCO  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                      1.2E+04 2.640  4.980  1000.0  2000.0
Glarborg, et al. 1986                      1.4E+04 2.640  4.980  1000.0  2000.0
Seeker, et al. 1985                        1.3E+11 0.500  6.810  1000.0  2000.0

 1CHN  + 1O            = 1NH   + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985                      5.2E+03 2.640  4.980  1000.0  2000.0
Glarborg, et al. 1986                      3.5E+03 2.640  4.980  1000.0  2000.0

 1CN   + 1HO           = 1NCO  + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                      5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986                      6.0E+13 0.000  0.000  1000.0  2000.0
Seeker, et al. 1985                        6.2E+13 0.000  0.000  1000.0  2000.0

 1C2N2 + 1HO           = 1HOCN + 1CN
Forward Rate Parameters:
Glarborg, et al. 1986                      1.9E+11 0.000  2.900  1000.0  2000.0

 1CH2  + 1NO           = 1HCNO + 1H
Forward Rate Parameters:
Glarborg, et al. 1986                      1.4E+12 0.000 -1.100  1000.0  2000.0

 1CH2  + 1NO           = 1CHN  + 1HO   +
Forward Rate Parameters:
```

```
This work                                   4.96E12 0.000 -1.100  1000.0  2000.0

 1CH2  + 1NO          = 1CH2O + 1N
Forward Rate Parameters:
Glarborg, et al. 1986                       1.6E+12 0.000  7.000  1000.0  2000.0

 1CH   + 1NO          = 1CHN  + 1O
Forward Rate Parameters:
Glarborg, et al. 1985                       1.1E+14 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                         1.0E+13 0.000  0.000  1000.0  2000.0
This work                                   1.0E+14 0.000  0.000  1000.0  2000.0

 1CH   + 1NO          = 1CHO  + 1N
Forward Rate Parameters:
Seeker, et al. 1985                         1.0E+14 0.000  0.000  1000.0  2000.0
This work                                   1.0E+13 0.000  0.000  1000.0  2000.0

 1CHO  + 1N           = 1CHN  + 1O
Forward Rate Parameters:
Seeker, et al. 1985                         1.0E+14 0.000  0.000  1000.0  2000.0

 1NCO  + 1H           = 1NH   + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985                       5.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                         5.0E+11 0.500  6.870  1000.0  2000.0

 1NCO  + 1NH2         = 1NH   + 1HNCO
Forward Rate Parameters:
Seeker, et al. 1985                         1.0E+11 0.500  5.000  1000.0  2000.0

 1NCO  + 1HO          = 1NO   + 1CO   + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                       1.0E+13 0.000  0.000  1000.0  2000.0
Glarborg, et al. 1986

 1NCO  + 1H2          = 1HNCO + 1H
Forward Rate Parameters:
Glarborg, et al. 1985                       8.6E+12 0.000  9.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                         3.0E+10 0.500  5.700  1000.0  2000.0

 1N    + 1CHCO        = 1CHN  + 1CO
Forward Rate Parameters:
Glarborg, et al. 1986                       5.0E+13 0.000  0.000  1000.0  2000.0

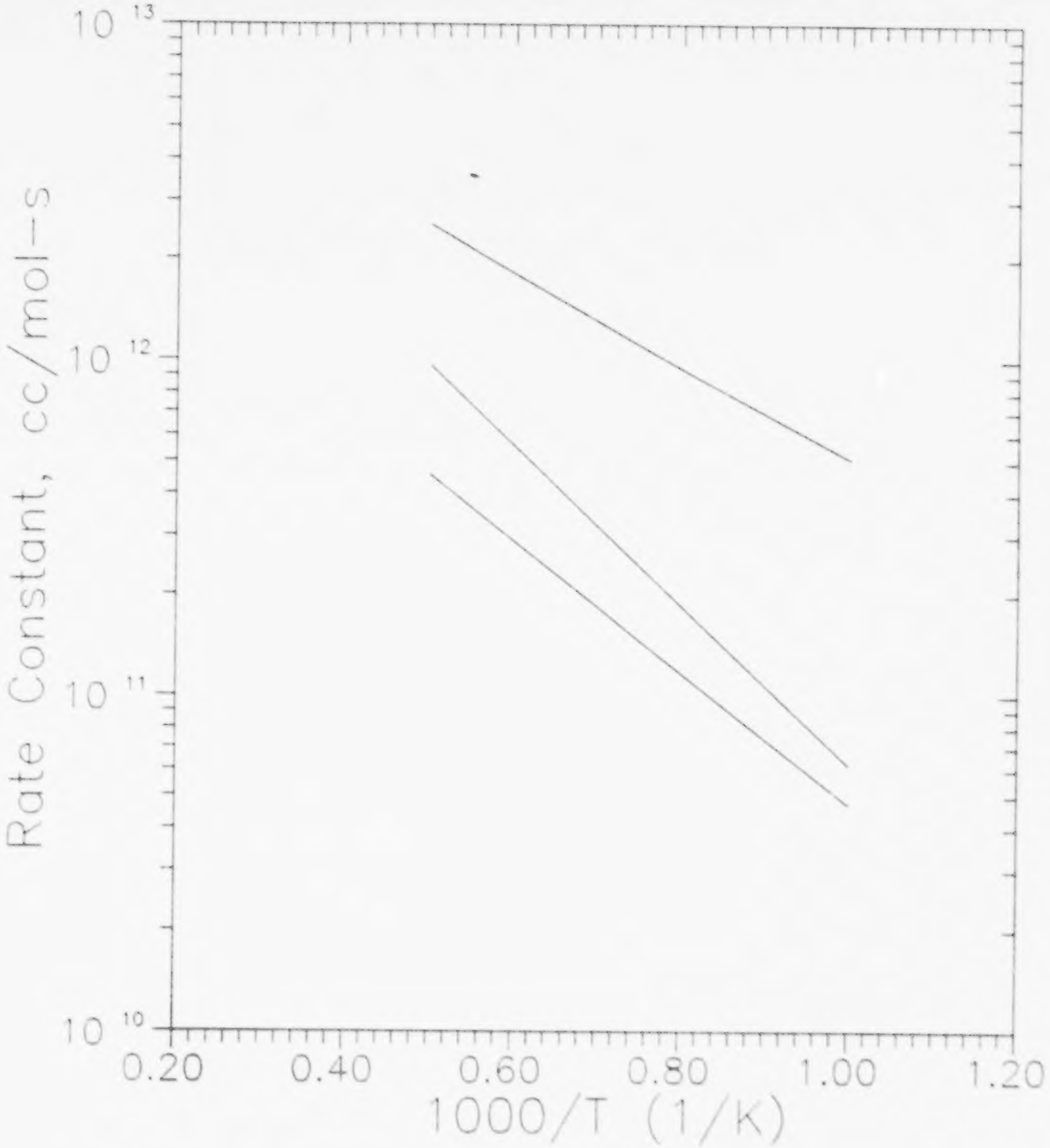
 1HNCO + 1H           = 1NH2  + 1CO
Forward Rate Parameters:
Glarborg, et al. 1985                       2.0E+13 0.000  3.000  1000.0  2000.0
Glarborg, et al. 1986
Seeker, et al. 1985                         5.0E+11 0.500  4.830  1000.0  2000.0

 1HNCO + 1HO          = 1NCO  + 1H2O
Forward Rate Parameters:
```

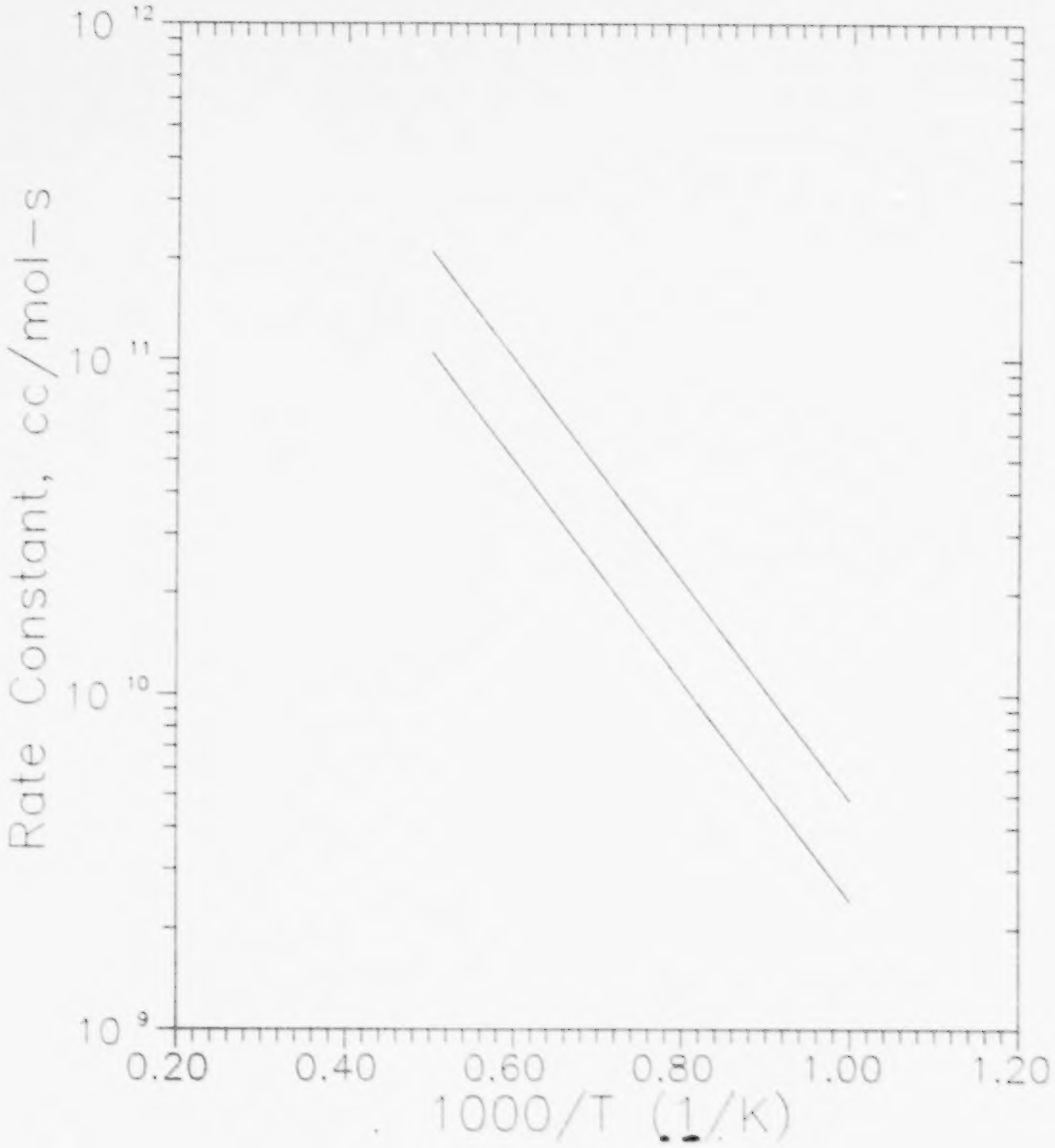
```
Seeker, et al. 1985                     1.0E+11 0.500  6.290  1000.0  2000.0

 1HCNO + 1H            = 1HCN  + 1HO
Forward Rate Parameters:
Glarborg, et al. 1986                   5.0E+13 0.000 12.000  1000.0  2000.0

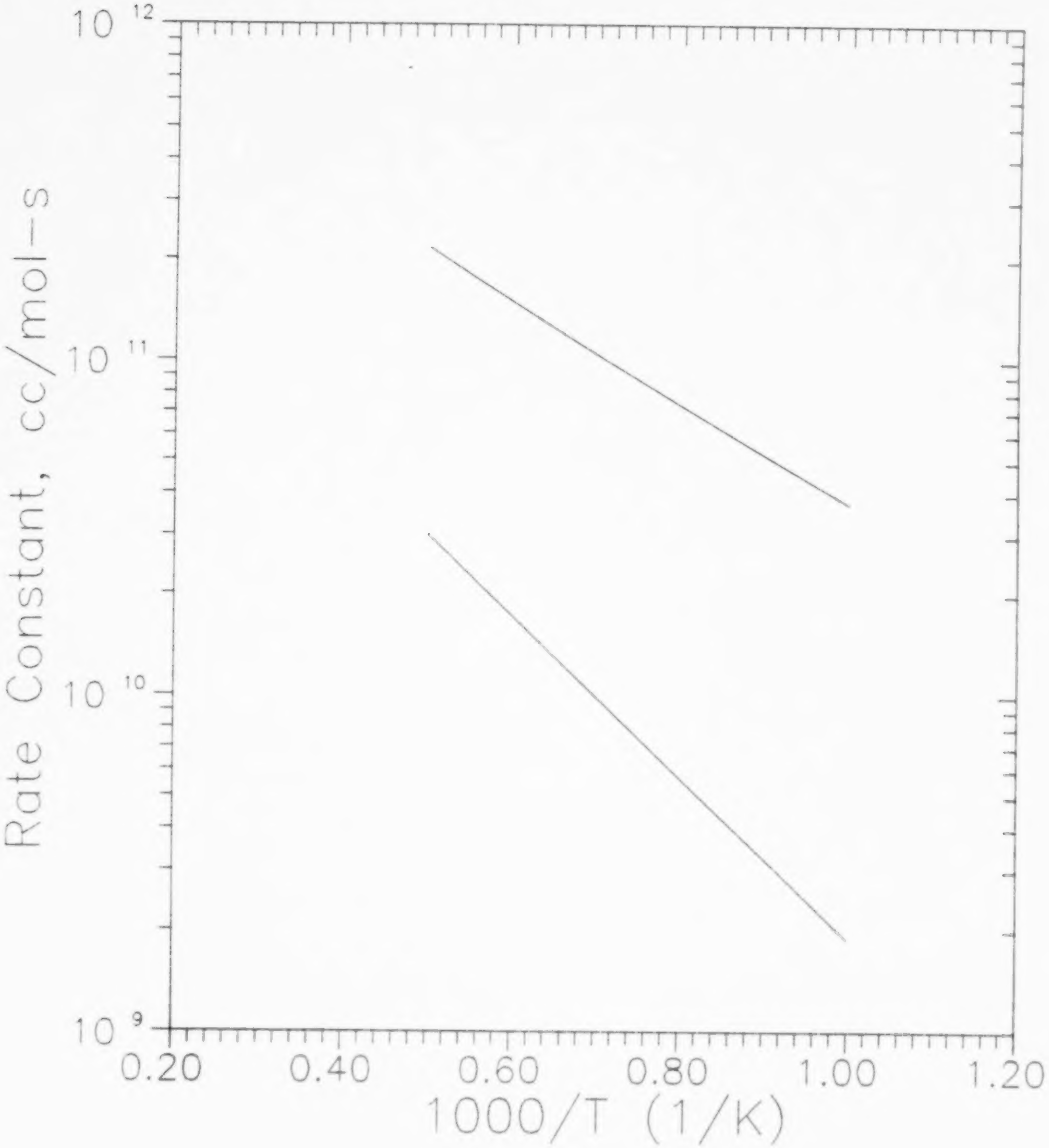
 1HOCN + 1H            = 1HNCO + 1H
Forward Rate Parameters:
Glarborg, et al. 1986                   1.0E+13 0.000  0.000  1000.0  2000.0
```


Rate Constant, cc/mol-s
10^13
10^12
10^11
10^10
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

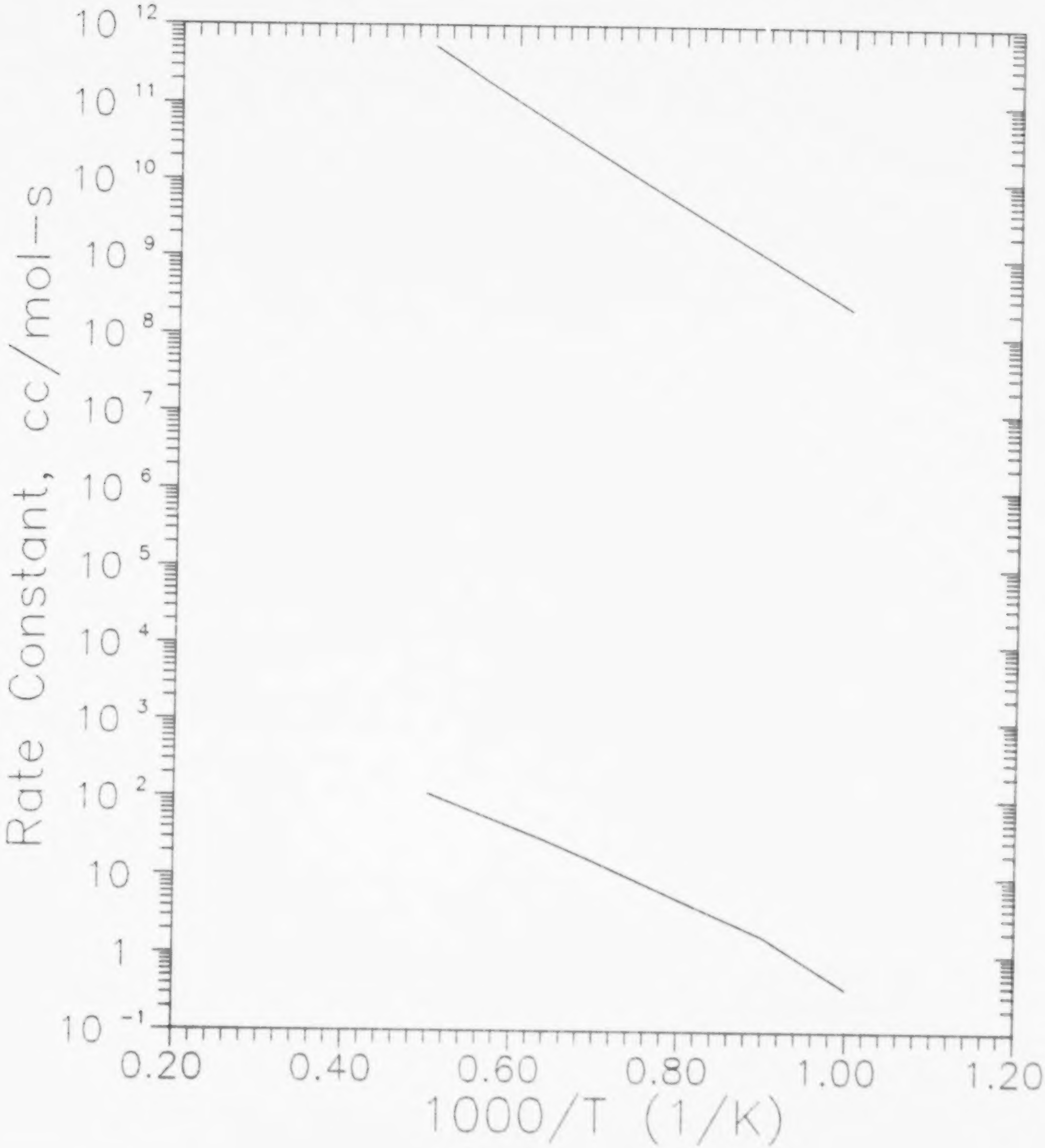
**CHN + HO = CN + H2O**


Rate Constant, cc/mol-s
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

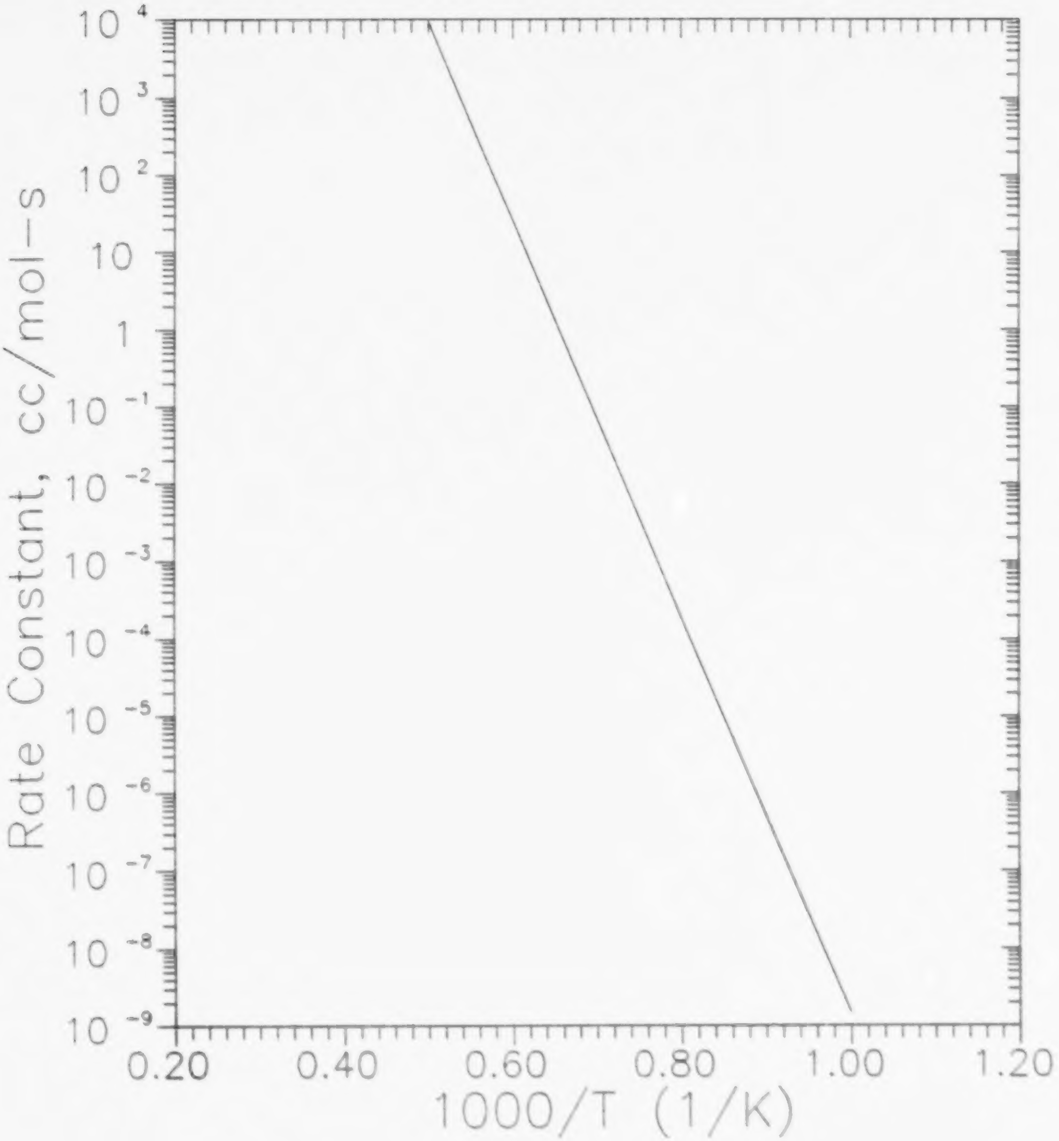
**CHN + HO = HOCN + H**


Rate Constant, cc/mol-s
$10^{12}$
$10^{11}$
$10^{10}$
$10^{9}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CHN + HO = HNCO + H**

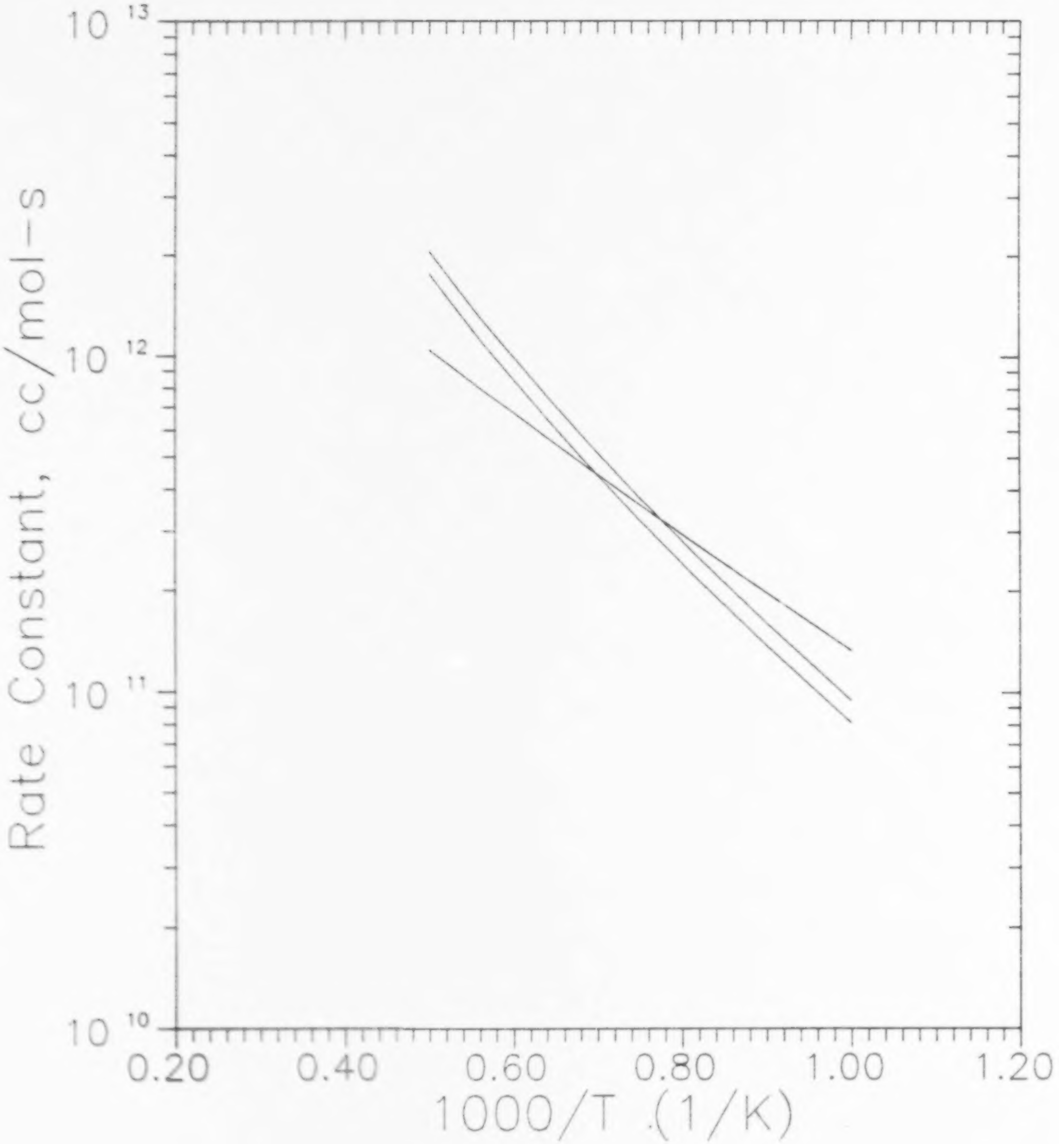

10 ¹²
10 ¹¹
10 ¹⁰
10 ⁹
10 ⁸
10 ⁷
10 ⁶
10 ⁵
10 ⁴
10 ³
10 ²
10
1
10 ⁻¹
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CHN + O = CN + HO**

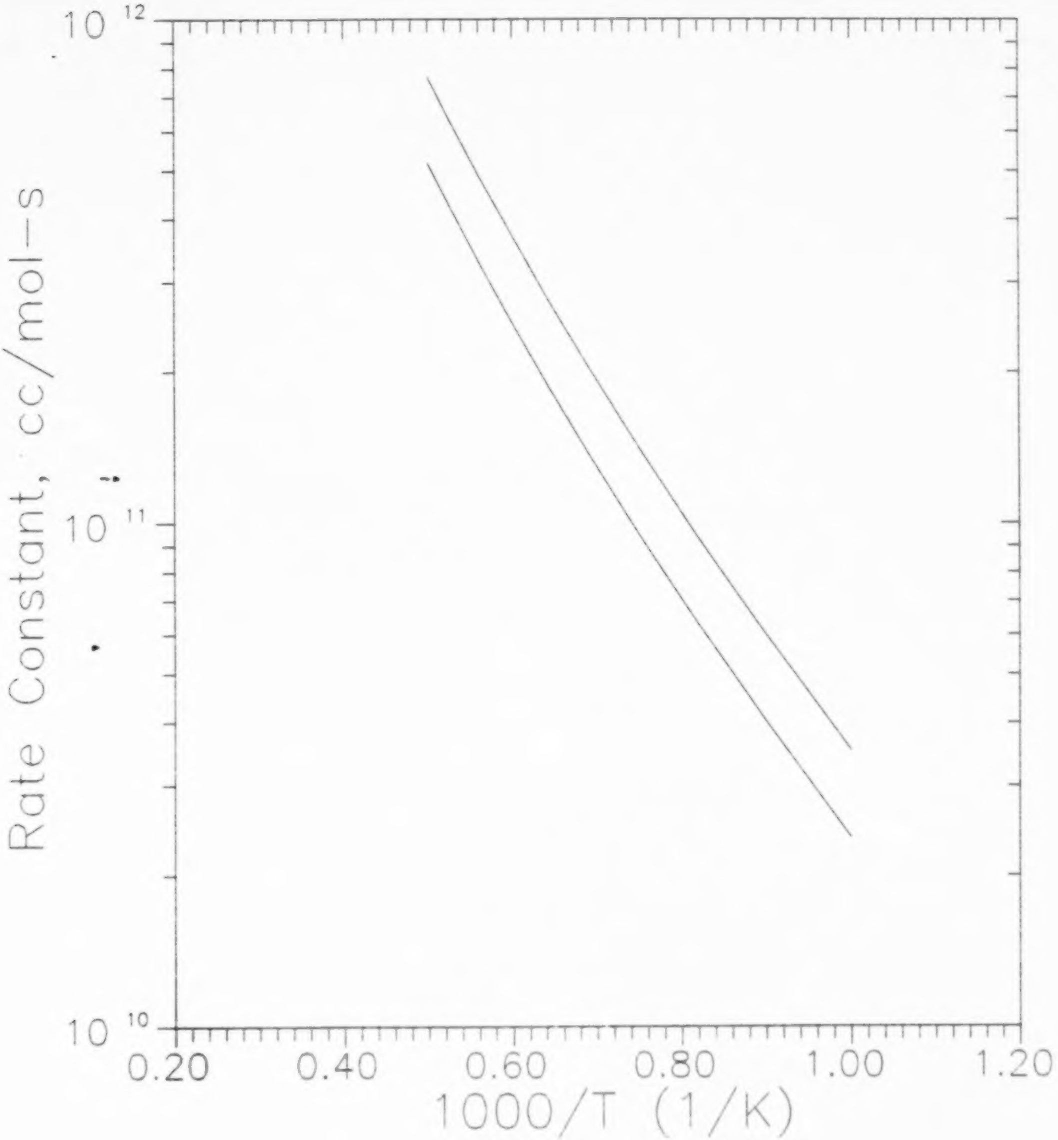


Rate Constant, cc/mol-s
$10^4$
$10^3$
$10^2$
10
1
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
$10^{-5}$
$10^{-6}$
$10^{-7}$
$10^{-8}$
$10^{-9}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

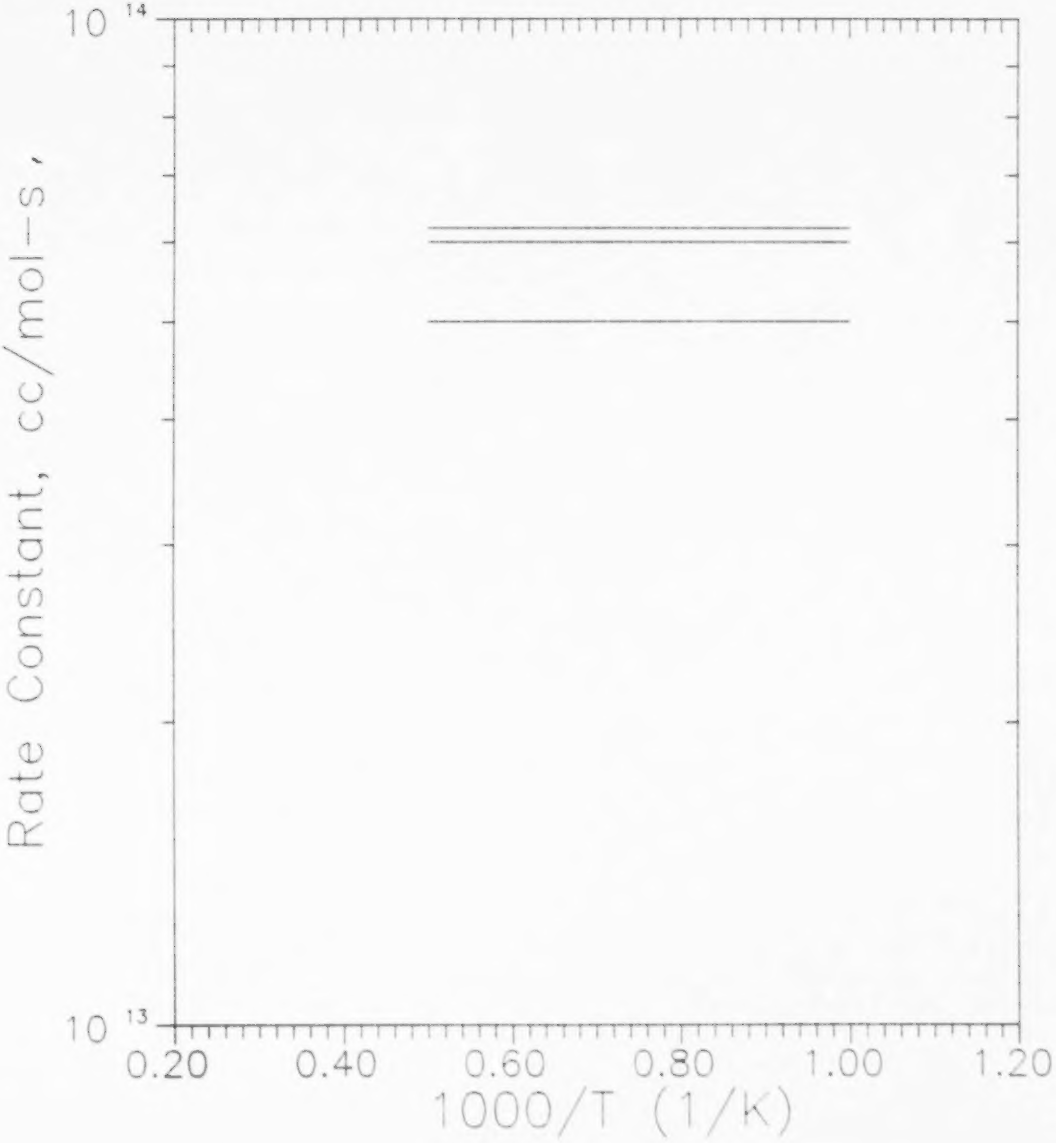
**CHN + O + M = CN + HO + M**


Rate Constant, cc/mol-s
10 13
10 12
10 11
10 10
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

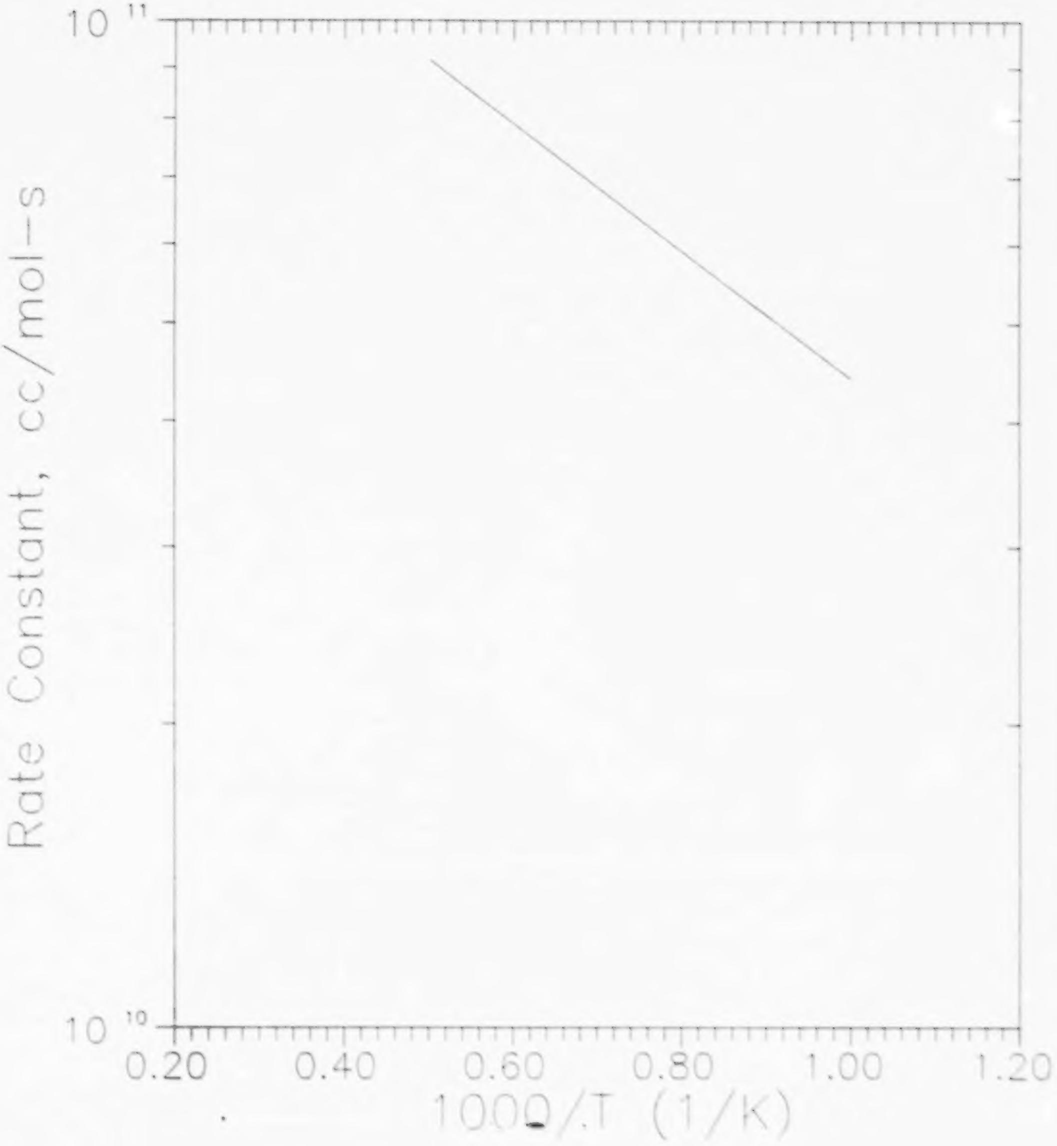
**CHN + O = NCO + H**


10 12
10 11
10 10
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

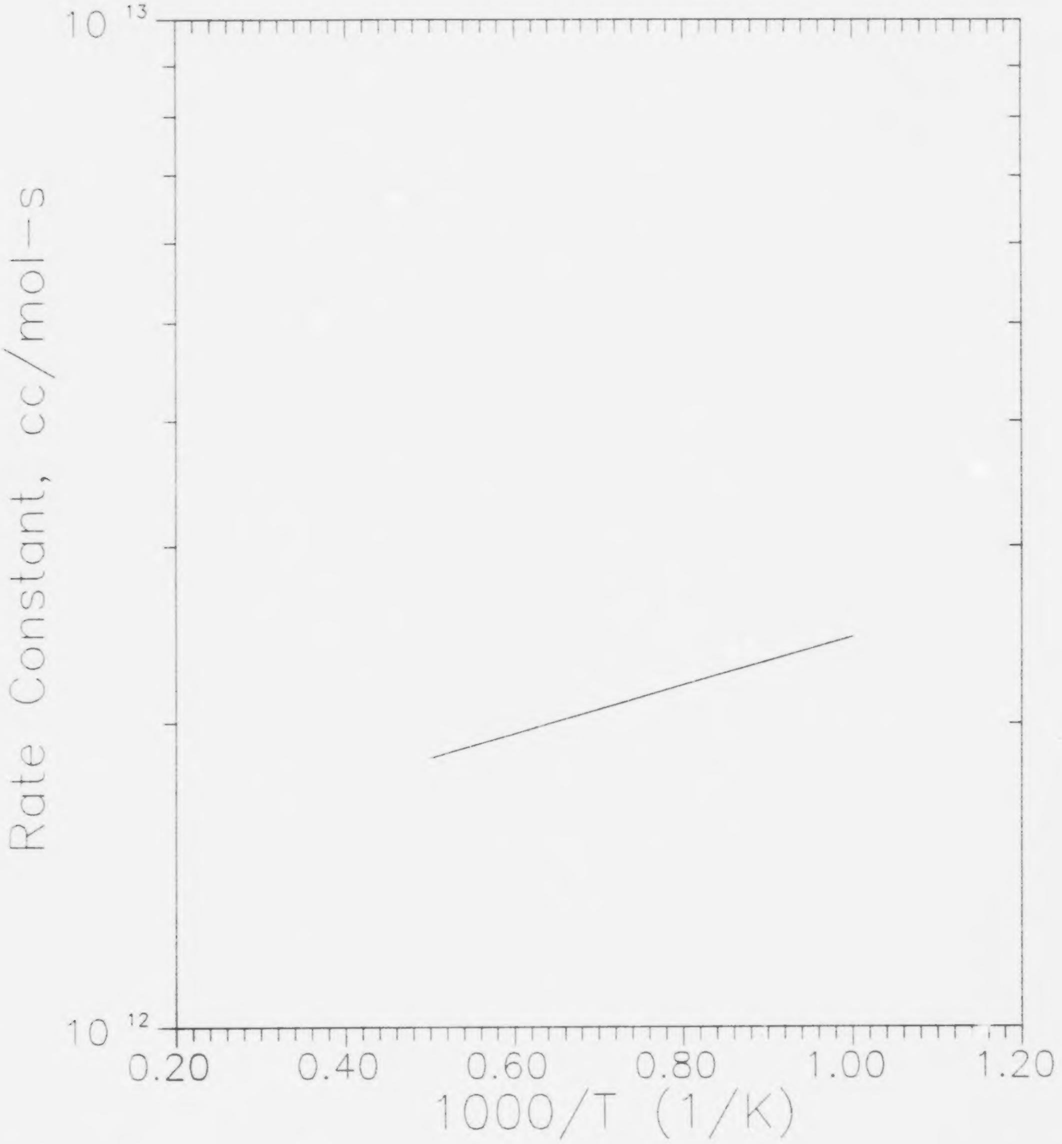
**CHN + O = NH + CO**


10 14
10 13
Rate Constant, cc/mol-s,
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CN + HO = NCO + H**

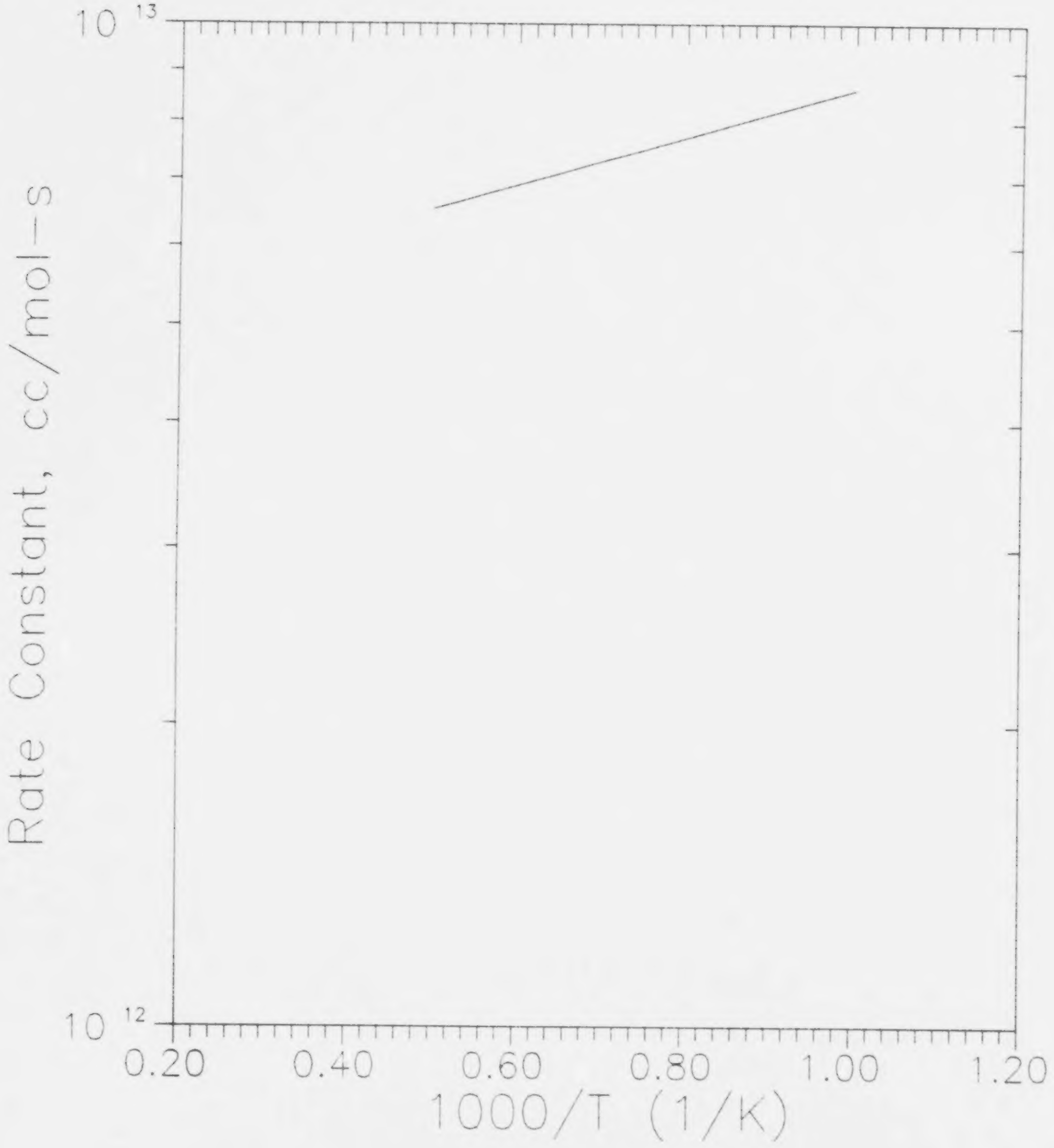


**C2N2 + HO = HOCN + CN**

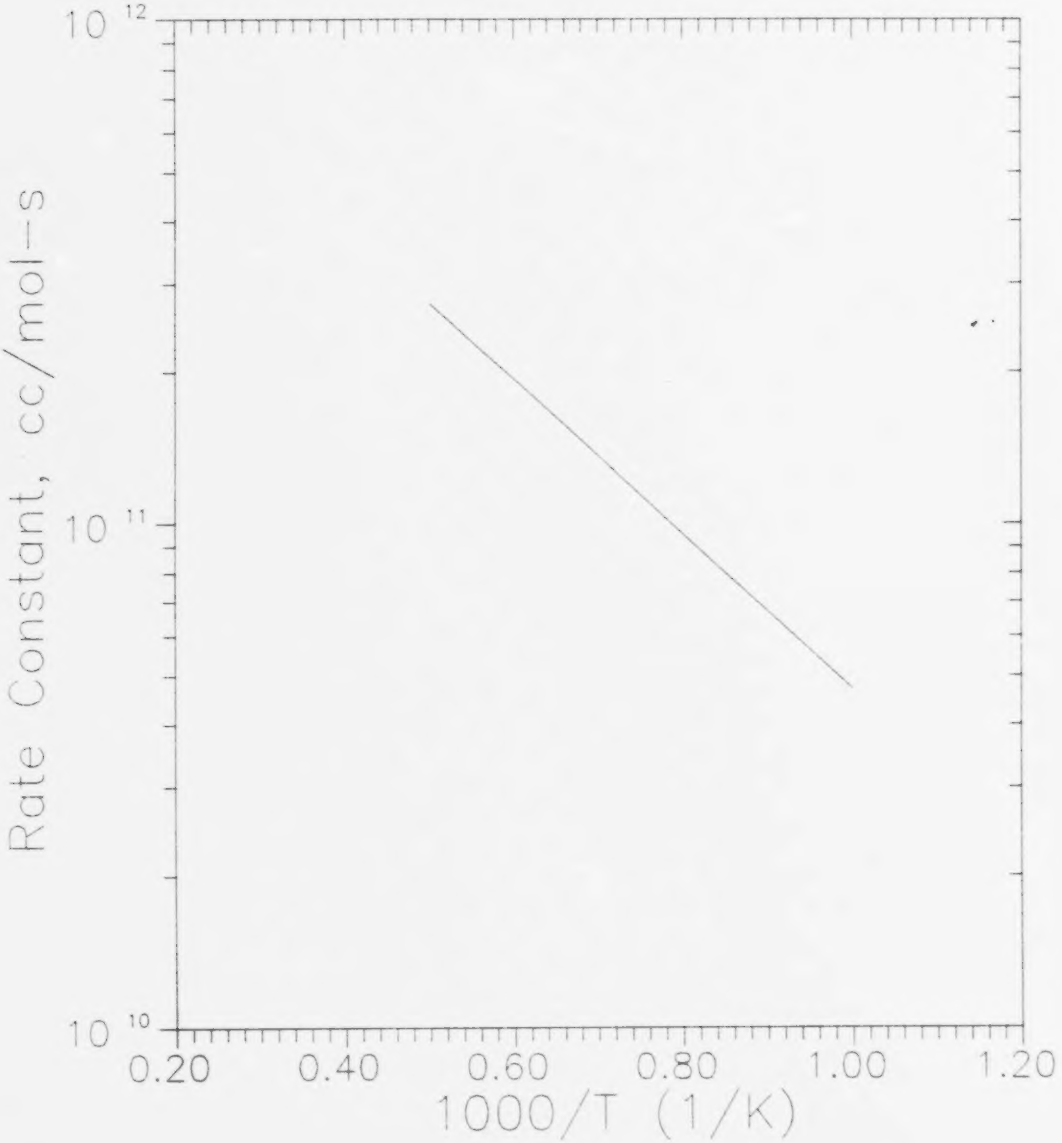


$10^{13}$
$10^{12}$
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

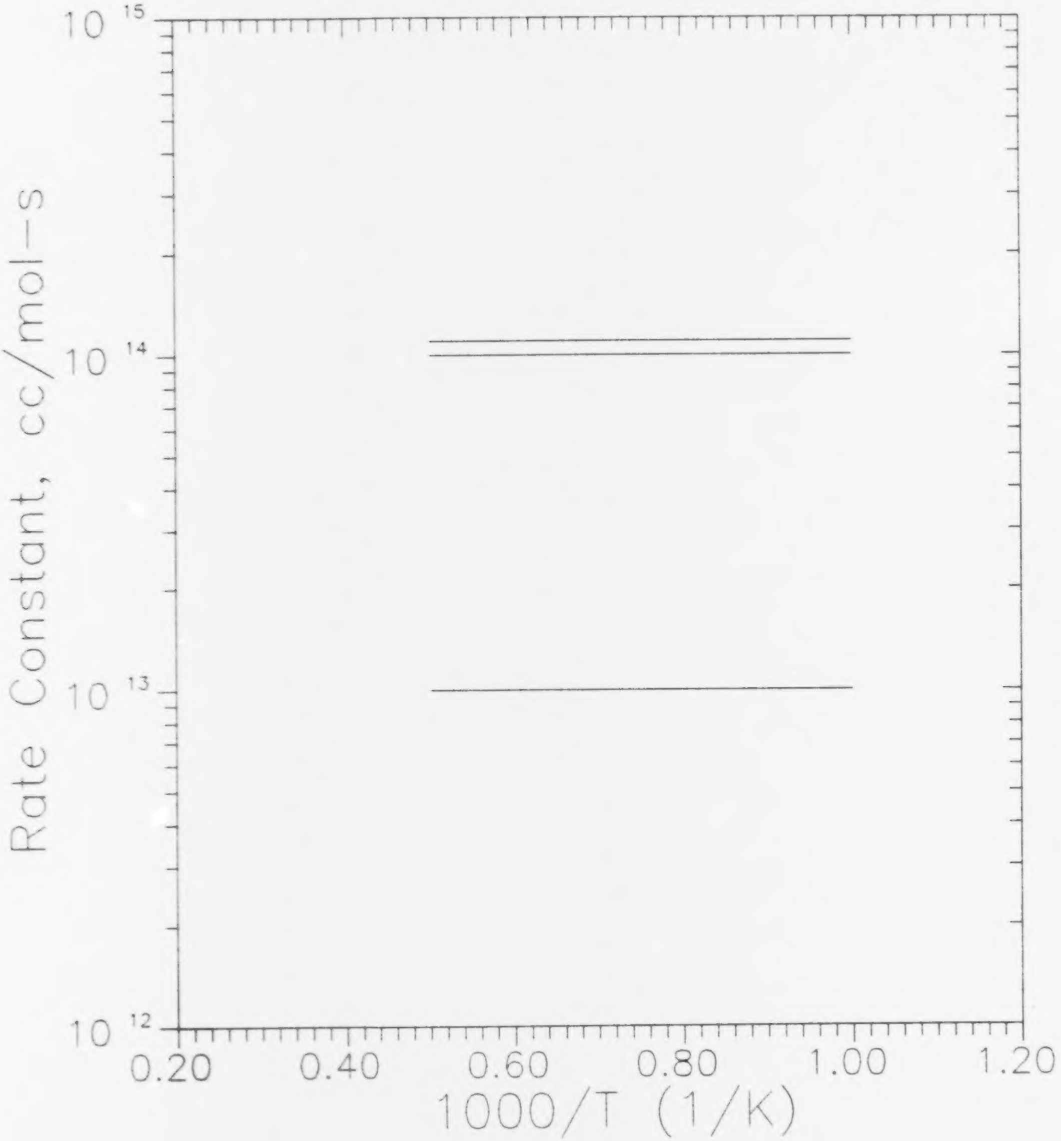
**CH2 + NO = HCNO + H**


10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + NO = CHN + HO**

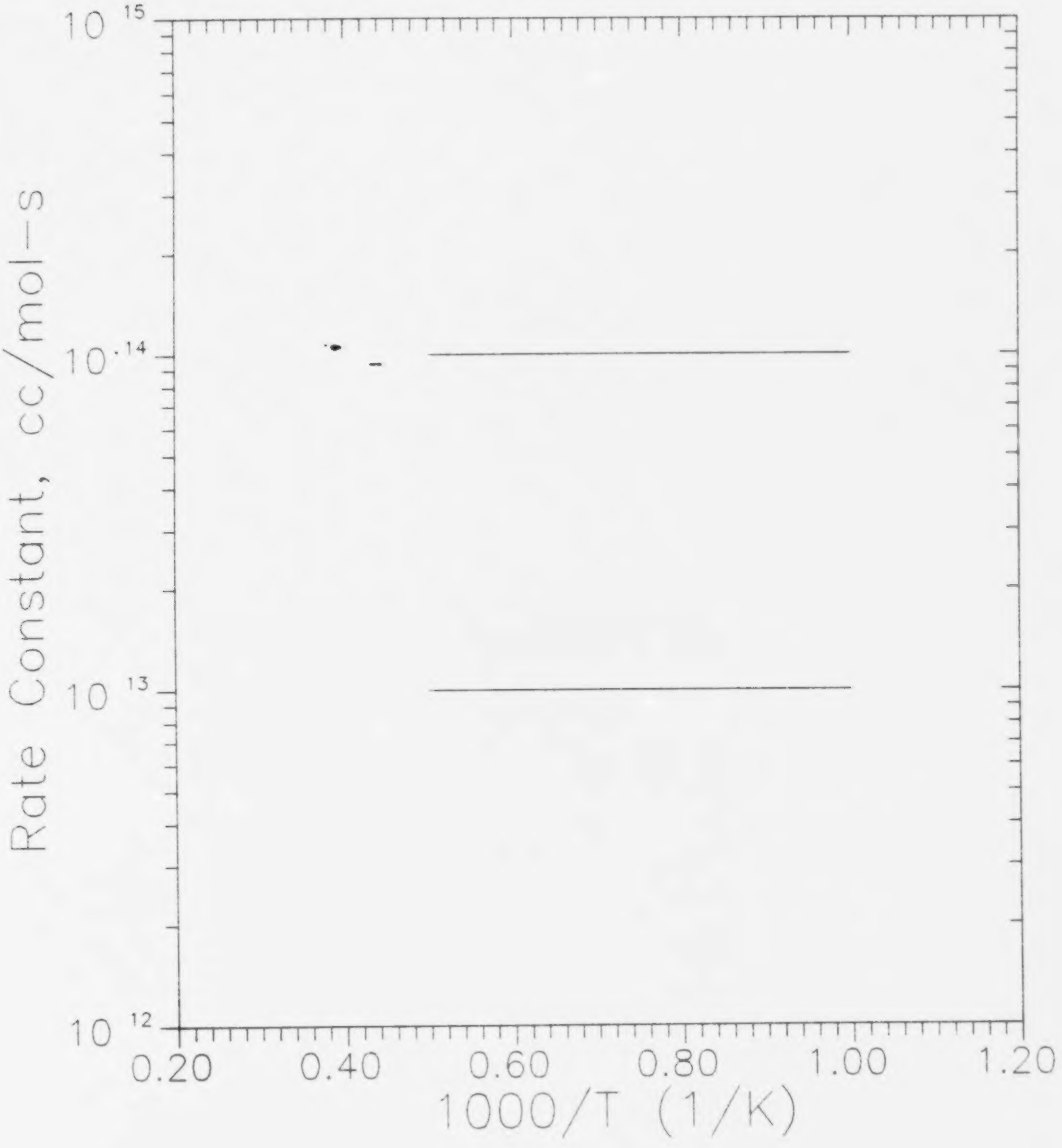

10^12
10^11
10^10
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**CH2 + NO = CH2O + N**



$10^{15}$
$10^{14}$
$10^{13}$
$10^{12}$
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

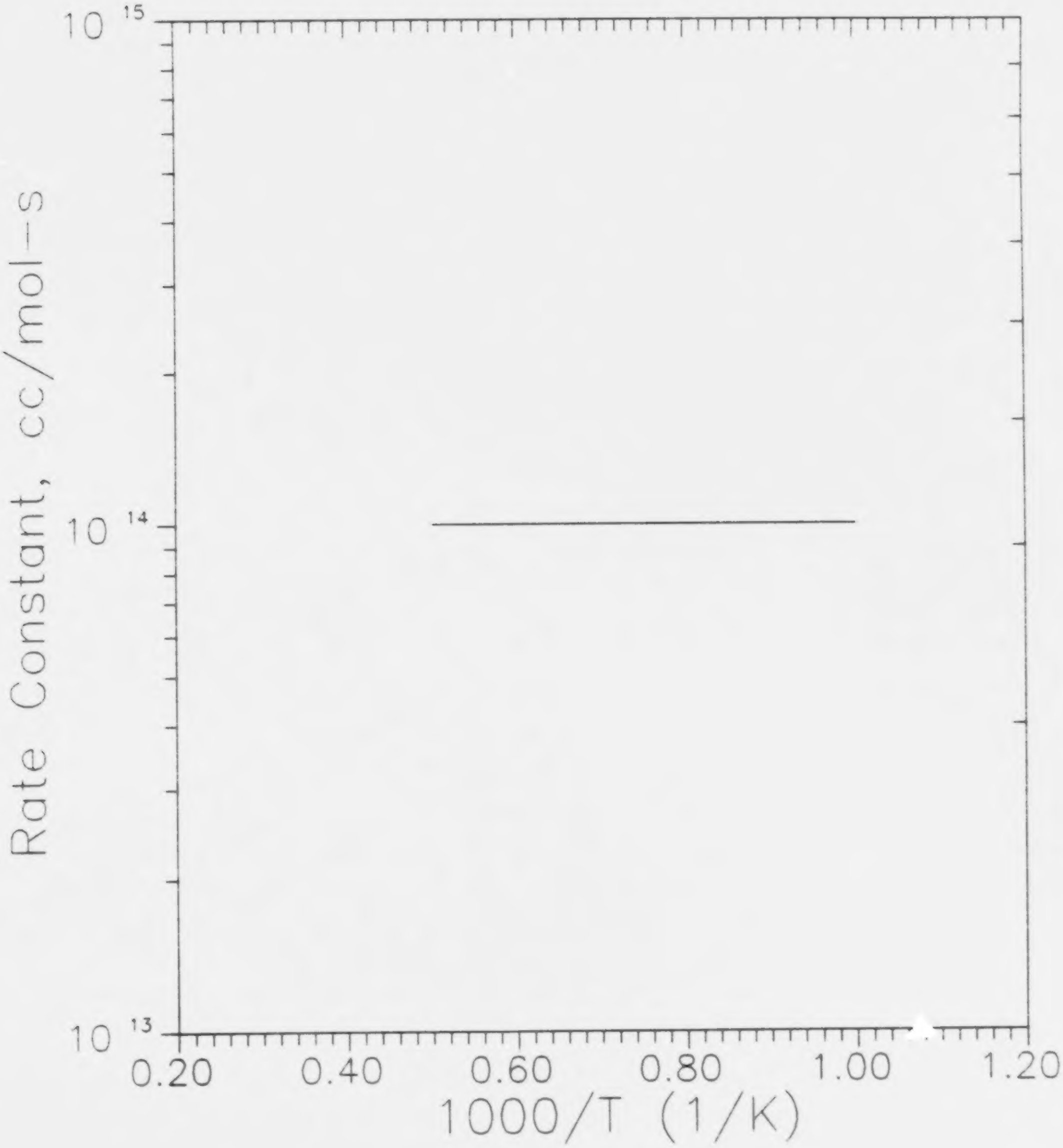
**CH + NO = CHN + O**



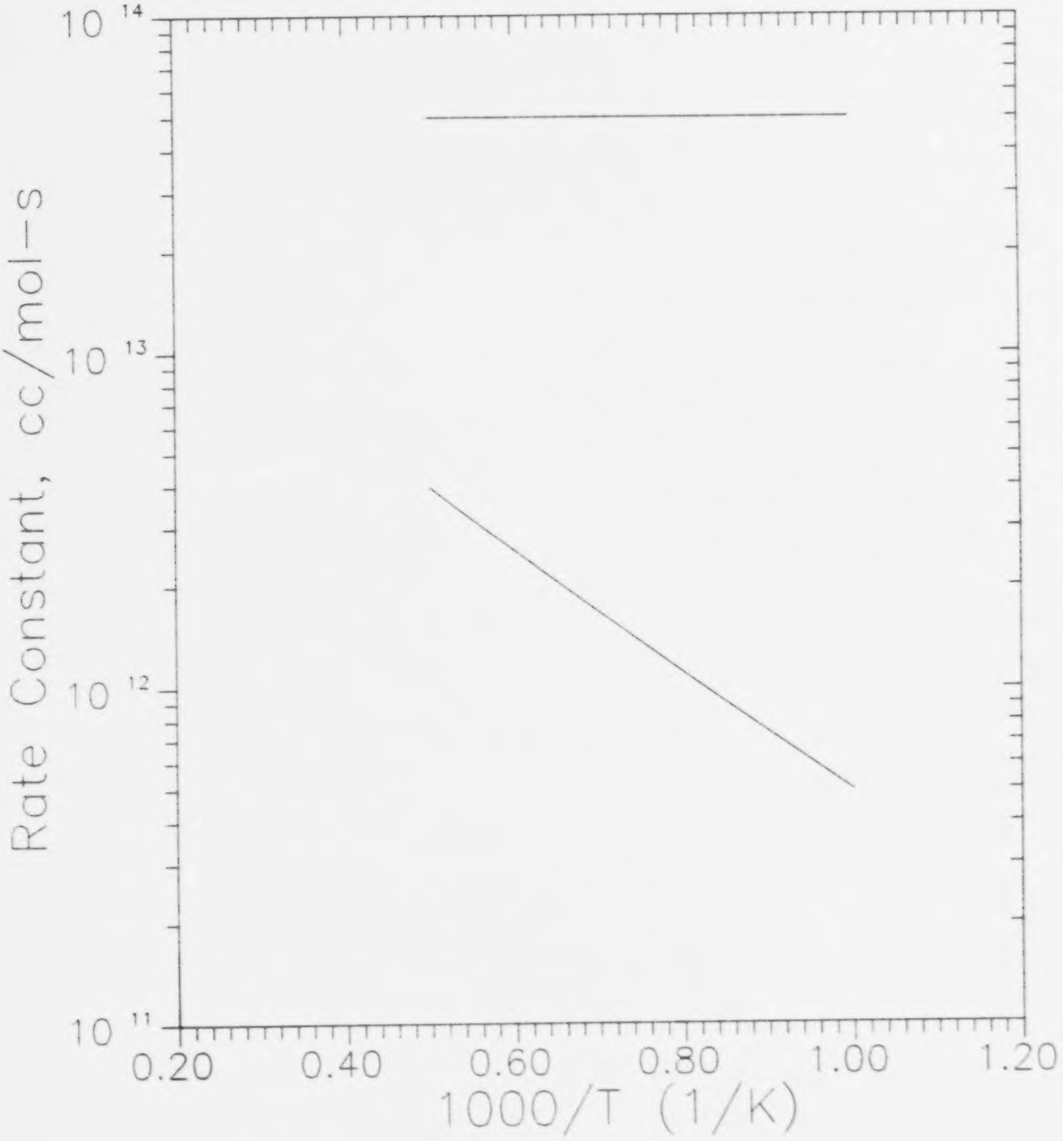
Rate Constant, cc/mol-s
1000/T (1/K)
$10^{15}$
$10^{14}$
$10^{13}$
$10^{12}$
0.20
0.40
0.60
0.80
1.00
1.20

**CH + NO = CHO + N**

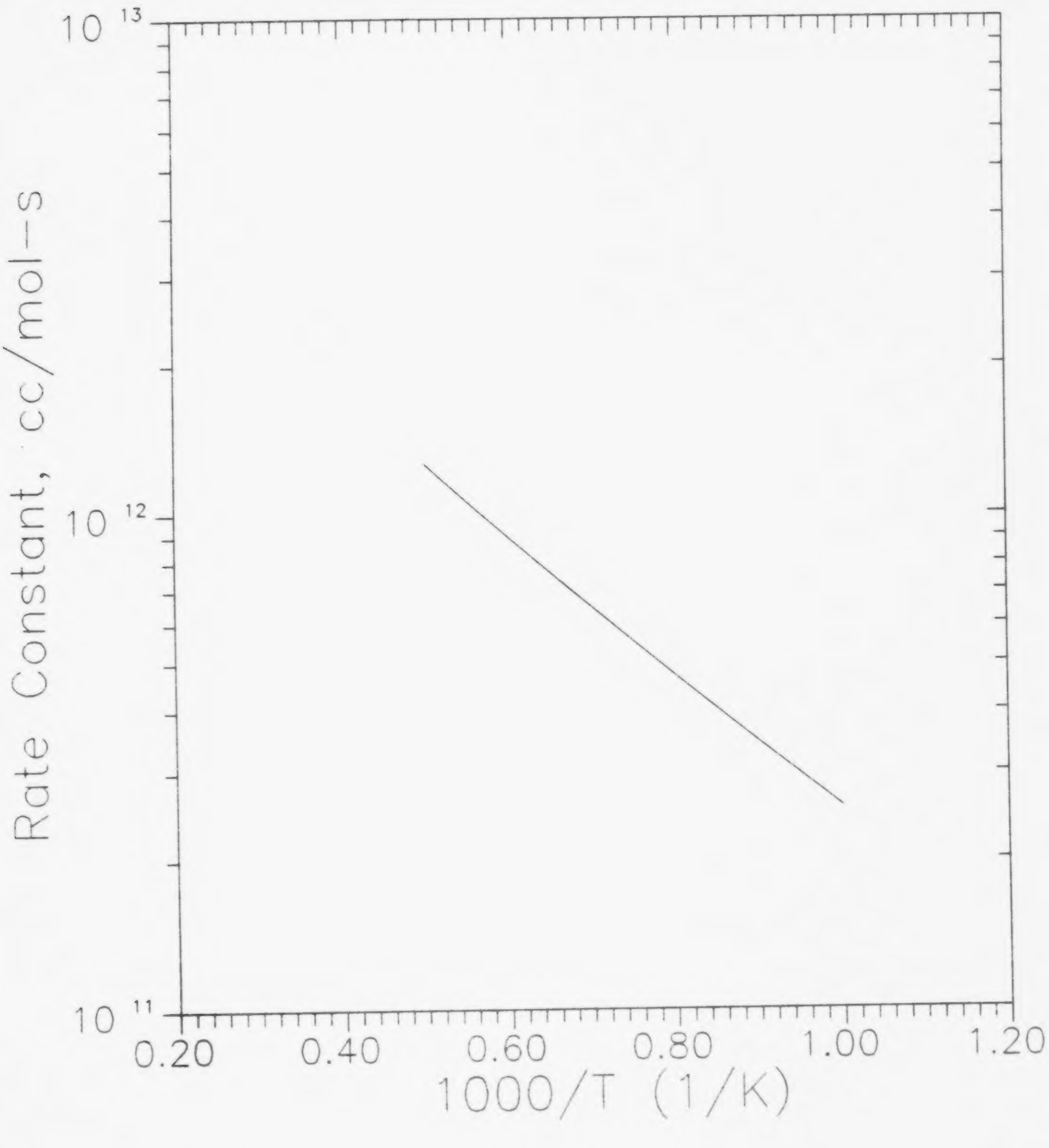
**CHO + N + = CHN + O +**



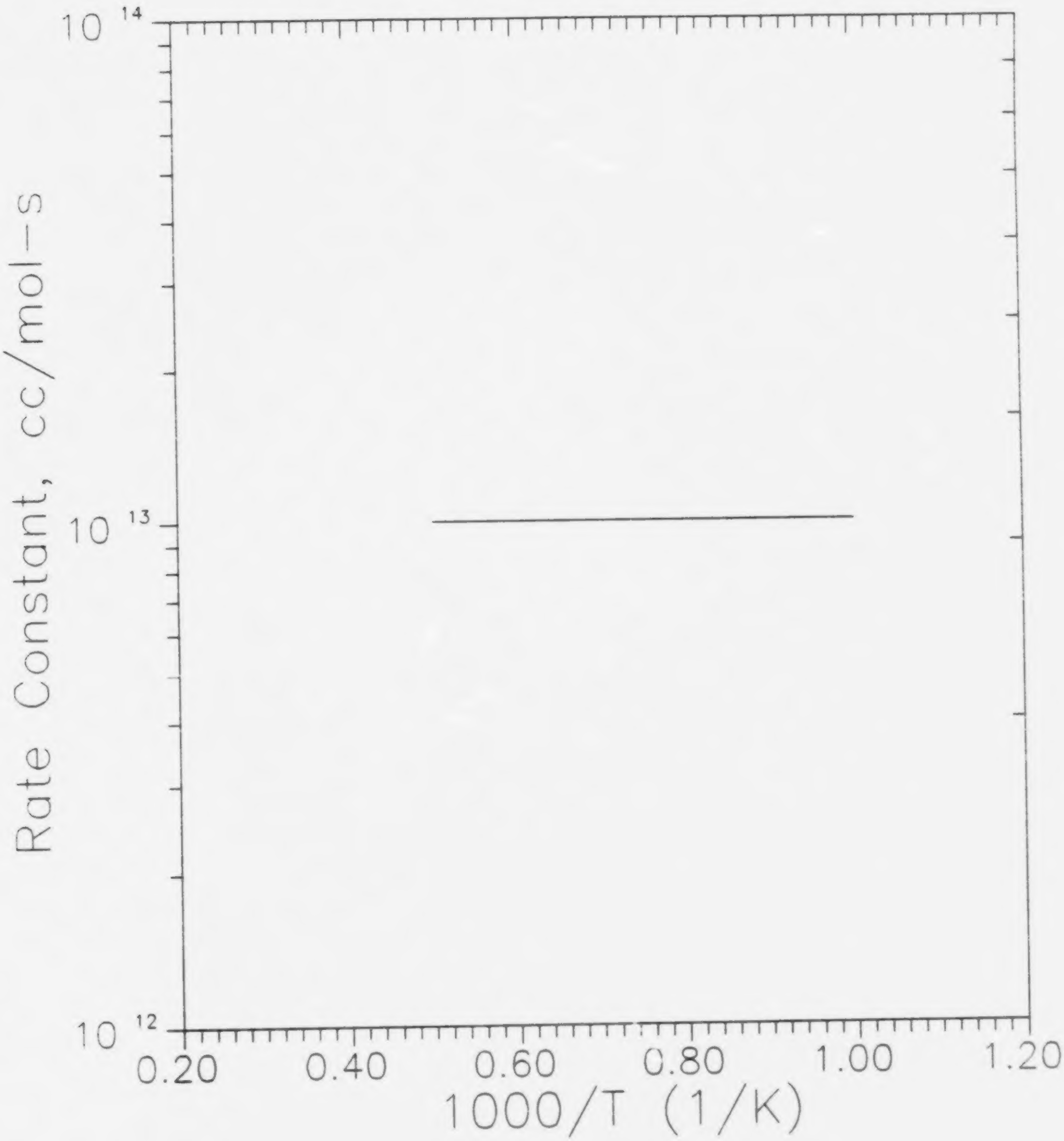
**CHO + N = CHN + O**


Rate Constant, cc/mol-s
10 14
10 13
10 12
10 11
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NCO + H = NH + CO**

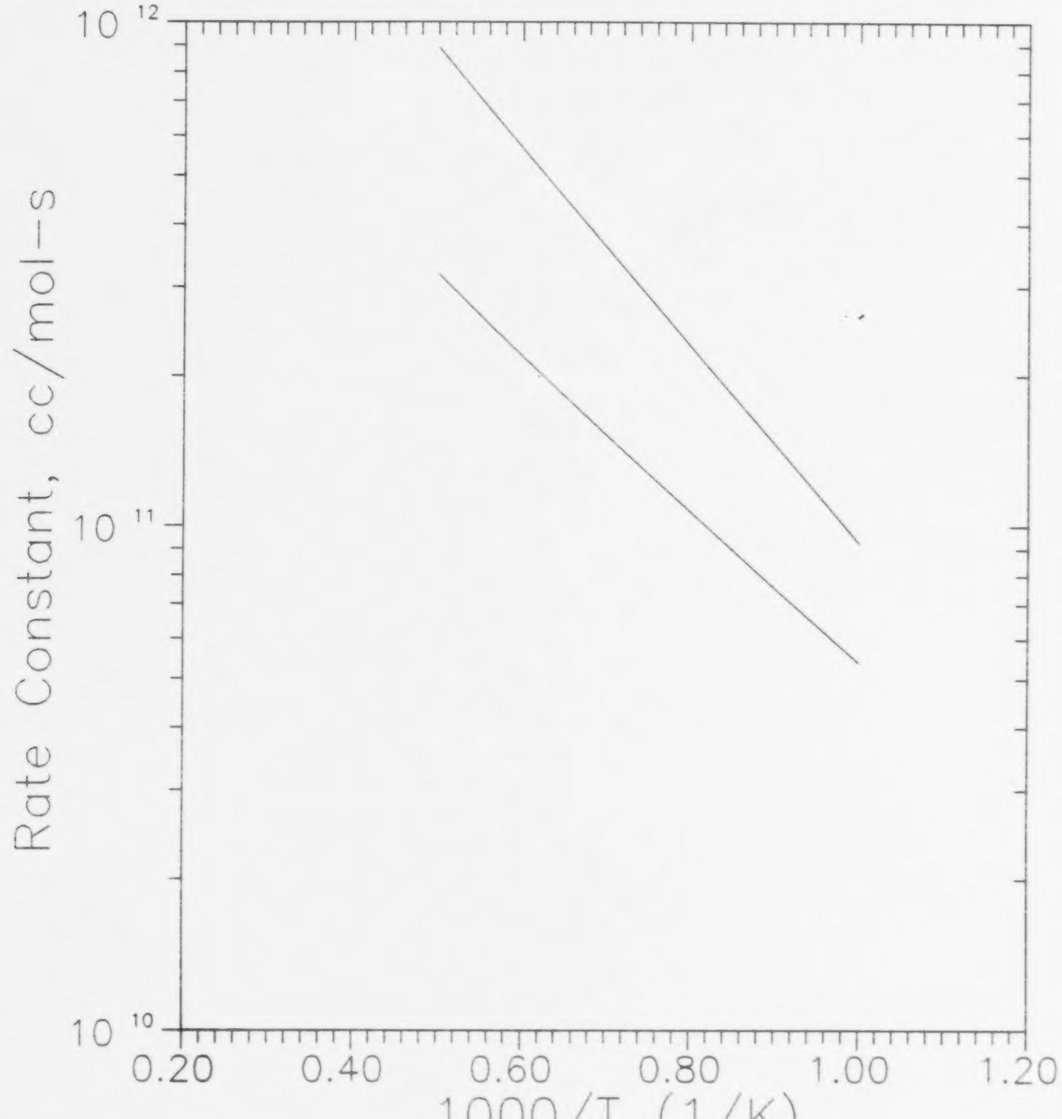


**NCO + NH2 = NH + HNCO**

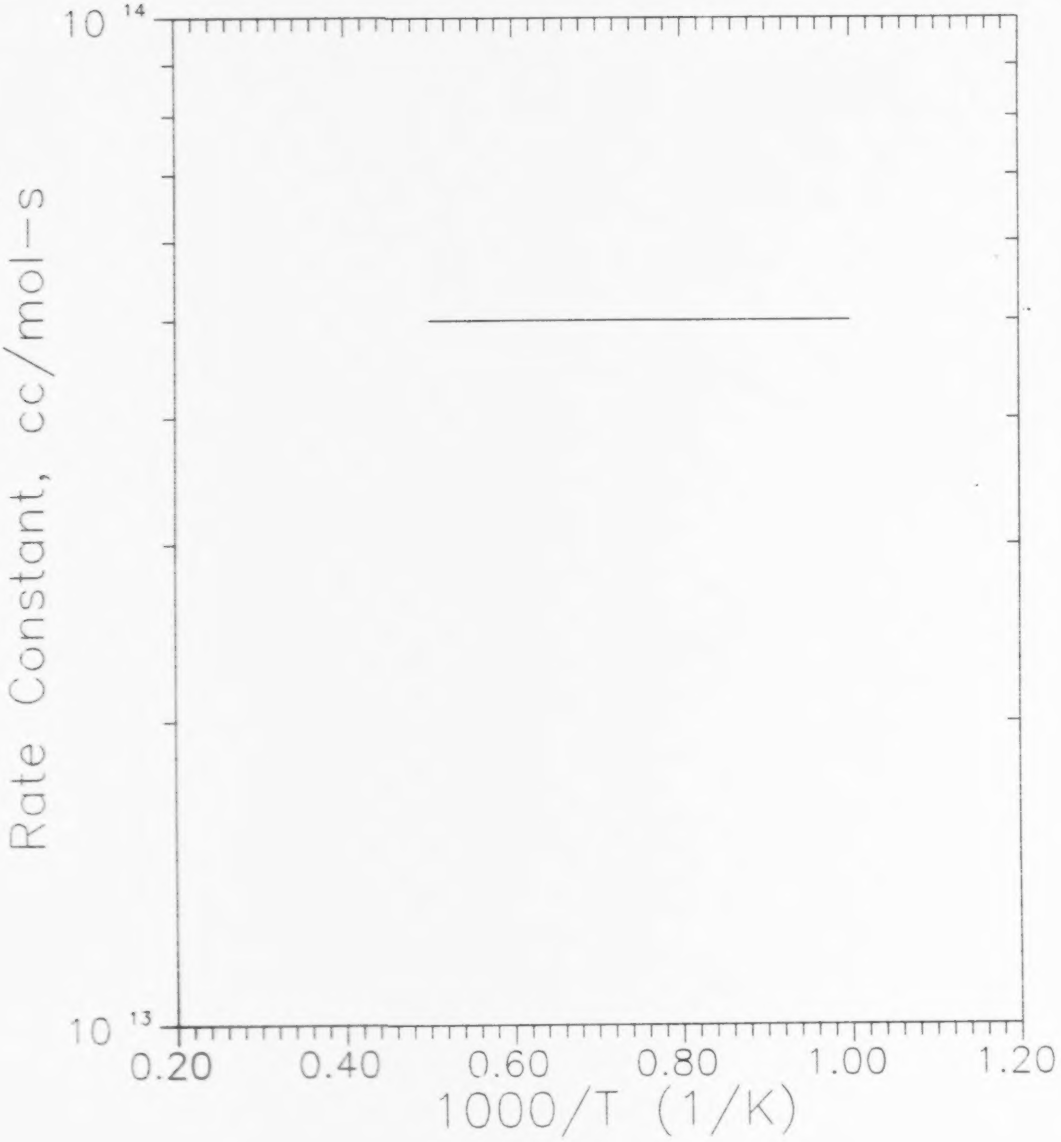


Rate Constant, cc/mol-s
$10^{14}$
$10^{13}$
$10^{12}$
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

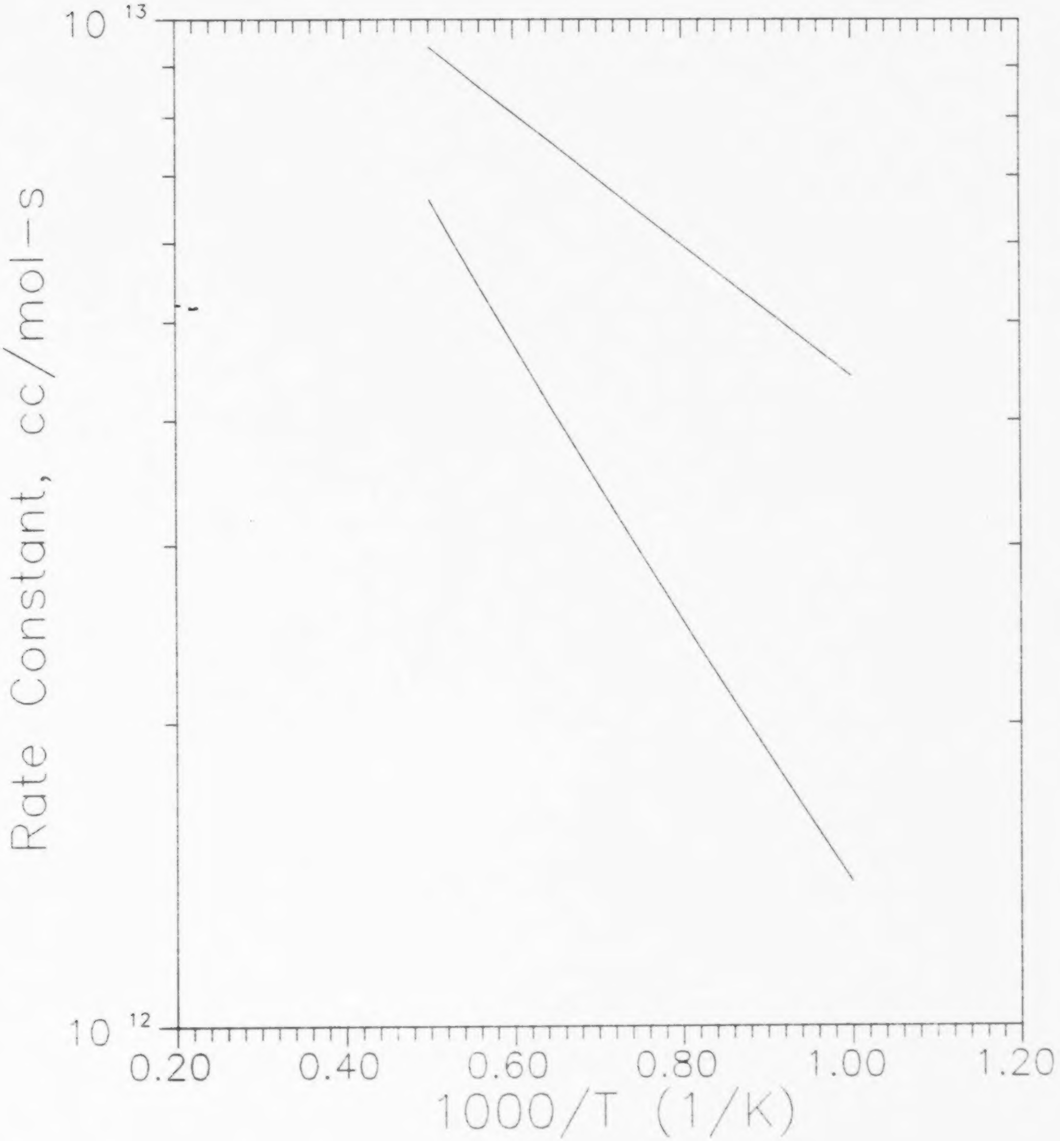
**NCO + HO = NO + CO + H**


10 12
10 11
10 10
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**NCO + H2 = HNCO + H**

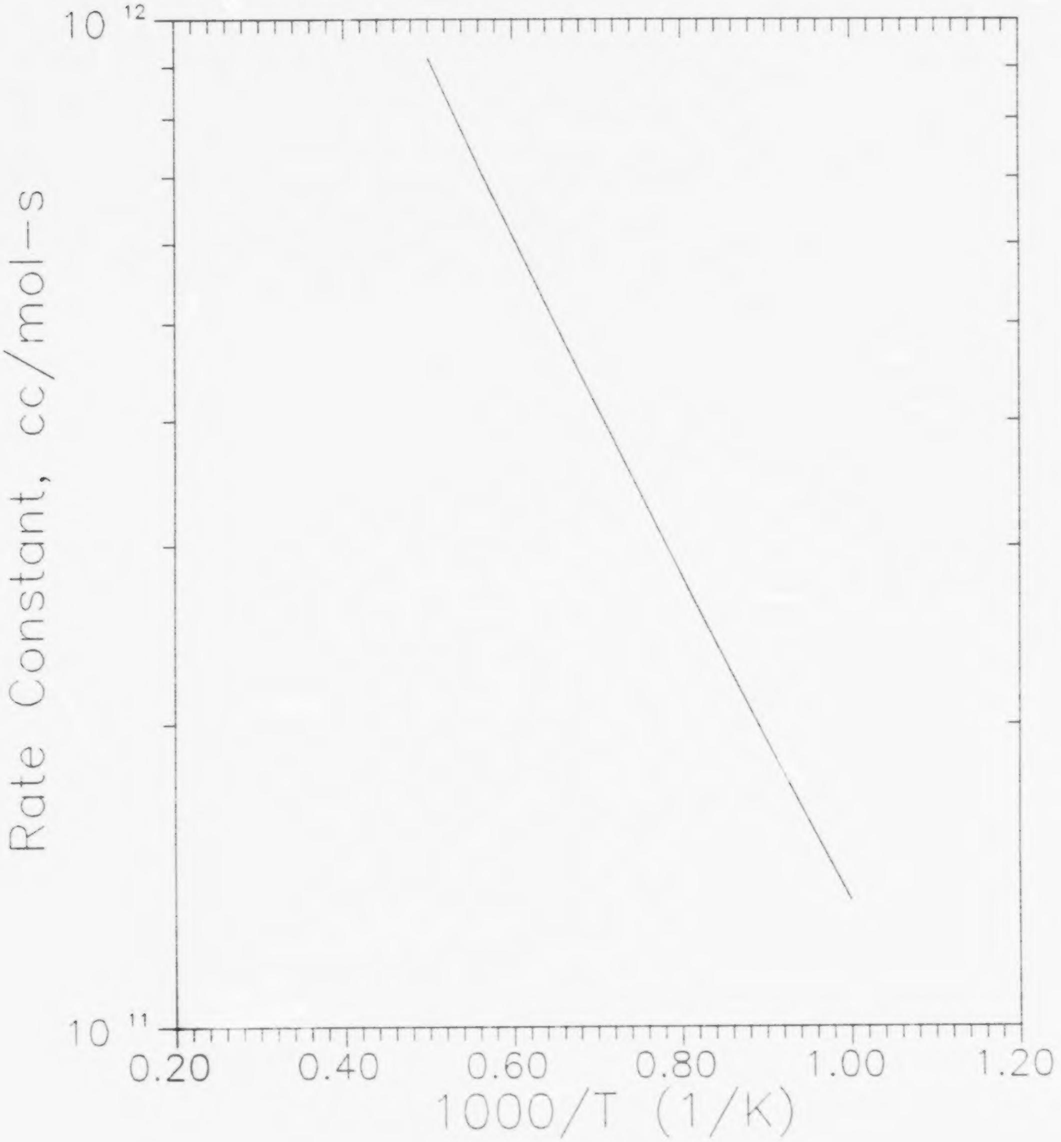

10 14
10 13
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)
Rate Constant, cc/mol-s

N + CHCO = CHN + CO

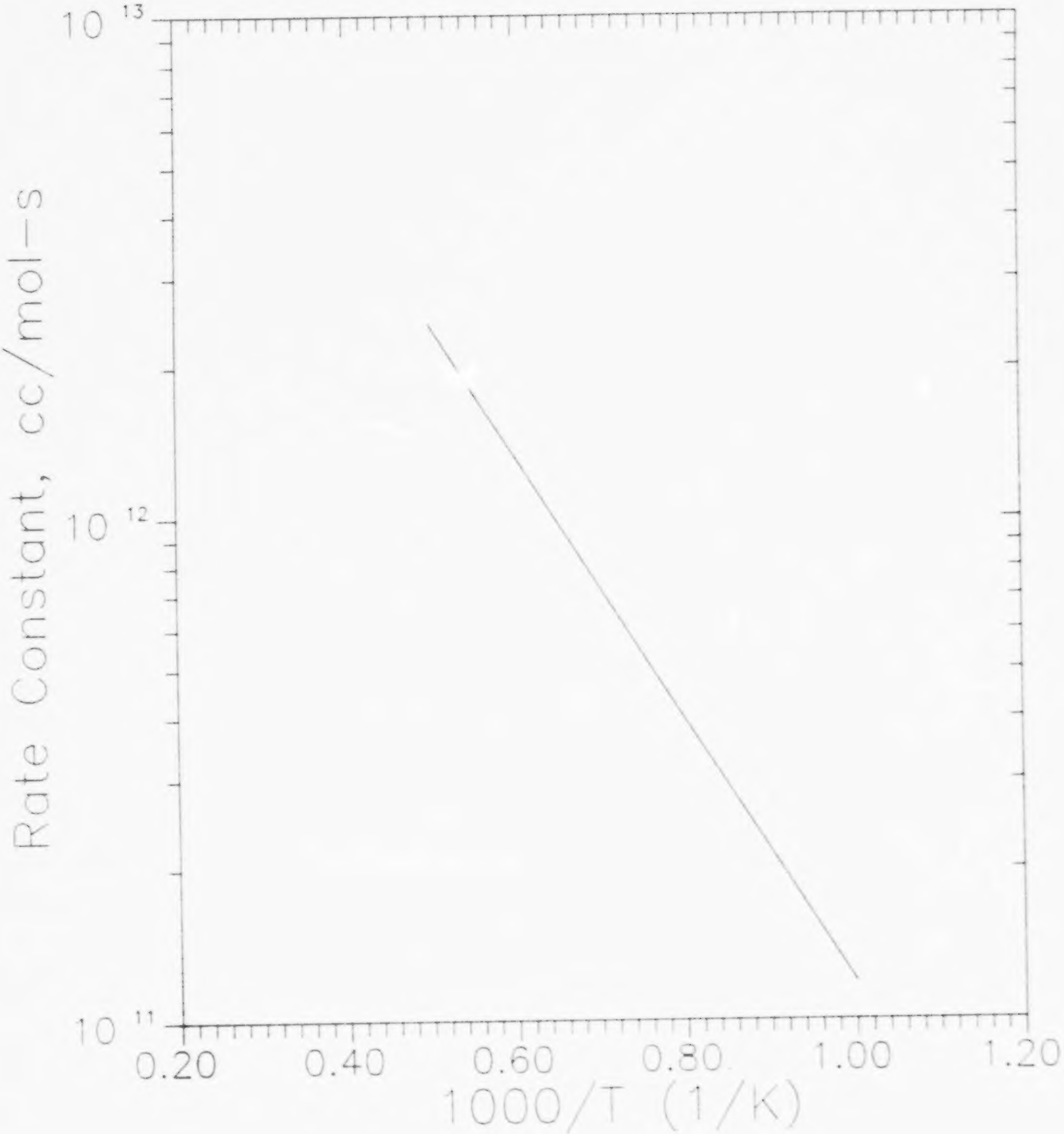


10 13
10 12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

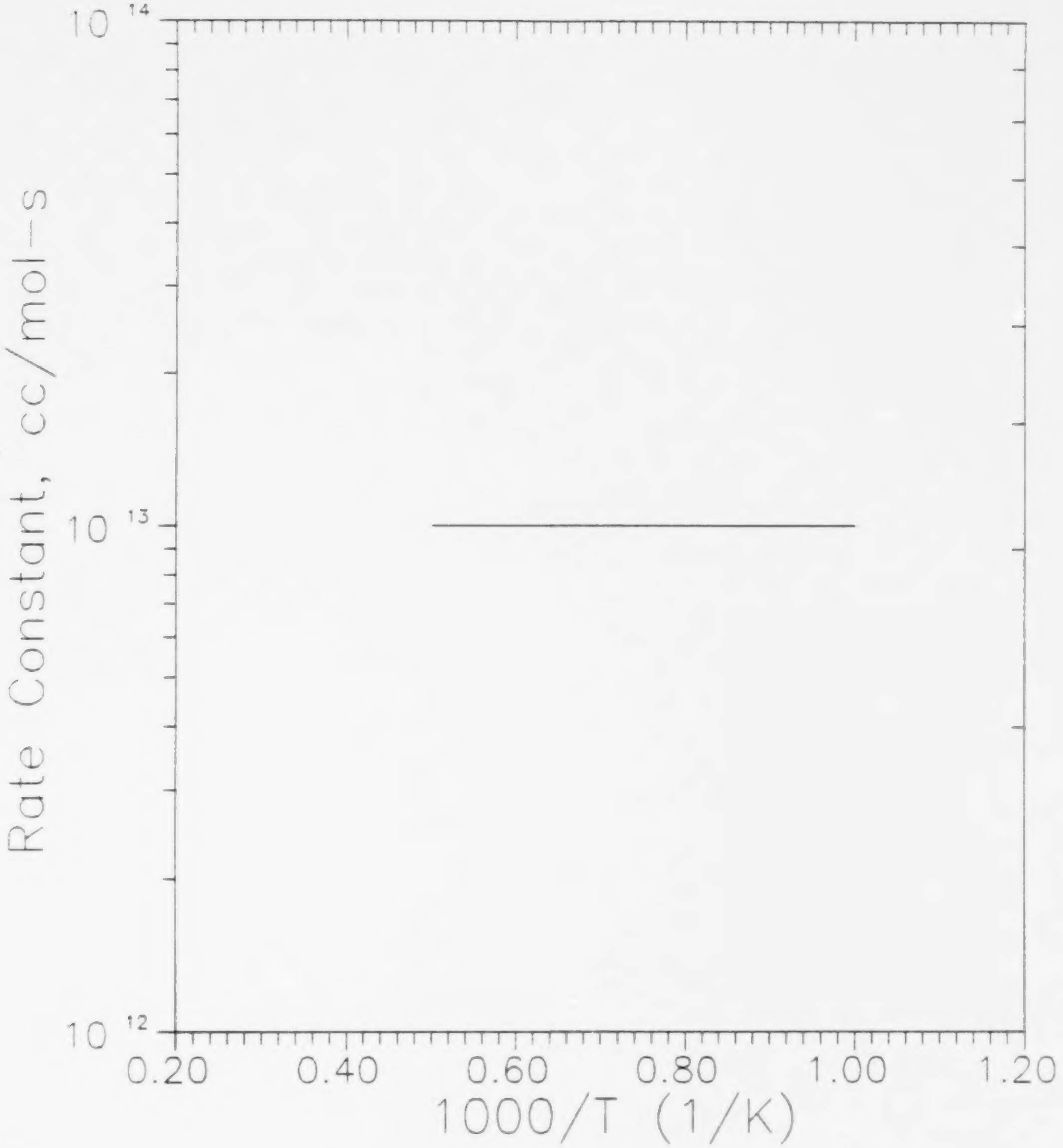
HNCO + H = NH2 + CO



**HNCO + HO = NCO + H2O**


10^13
10^12
10^11
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HCNO + H = HCN + HO**


10^14
10^13
10^12
Rate Constant, cc/mol-s
0.20
0.40
0.60
0.80
1.00
1.20
1000/T (1/K)

**HOCN + H = HNCO + H**

# APPENDIX B
# THERMODYNAMIC DATA

In the following tables are listed the thermodynamic data used by the one-dimensional flame code for the calculation of reverse rates of the reactions listed in Table 1 of the main report. Table B-1 lists the species, their heats of formation at 298 K, and their molecular weights. Table B-2 is a list of the following functions:

| | |
|---|---|
| H(T) - H(298) | (kcal/mol) |
| [F(T) - H(298)]/T | (cal/mol/K) |
| $C_p(T)$ | (cal/mol/K) |

where:

H represents enthalpy
F represents gibbs energy
$C_p$ is heat capacity

Fifty values are given for each function at intervals of 100 K starting at 100 K. The formula of the species and the function for which values are given are listed in the right hand columns of the table.

## TABLE B-1

## LIST OF SPECIES AND ENTHALPY AT 298 K

| Species | mol weight (g/g-mol) | Enthalpy of formation at 298 K (kcal/mol) |
|---|---|---|
| C | 12.011 | 171.290 |
| C2H | 25.032 | 134.003 |
| C2H2 | 26.041 | 54.194 |
| C2H3 | 27.051 | 68.410 |
| C2H4 | 28.061 | 12.538 |
| C2H5 | 29.070 | 28.015 |
| C2H6 | 30.080 | -20.041 |
| CH | 13.021 | 141.999 |
| CH2 | 14.030 | 92.484 |
| CH2O | 30.030 | -27.702 |
| CH3 | 15.040 | 34.820 |
| CH3O | 31.039 | 3.896 |
| CH4 | 16.050 | -17.898 |
| CN | 26.078 | 104.002 |
| CO | 28.010 | -26.417 |
| CO2 | 44.010 | -94.051 |
| H | 1.010 | 52.093 |
| H2 | 2.019 | 0.001 |
| H2O | 18.019 | -57.797 |
| H2O2 | 34.018 | -32.527 |
| CHN | 27.088 | 32.301 |
| CHO | 29.020 | 10.400 |
| HNCO | 43.087 | -24.895 |
| HNO | 31.076 | 23.799 |
| HO2 | 33.008 | 2.499 |
| HOCN | 43.087 | -2.280 |
| N | 14.067 | 112.950 |
| N2 | 28.134 | 0.000 |
| N2H2 | 30.153 | 50.898 |
| N2O | 44.133 | 19.612 |
| NCO | 42.077 | 38.101 |
| NH | 15.077 | 85.200 |
| NH2 | 16.086 | 45.501 |
| NH3 | 17.096 | -10.972 |
| HN2 | 29.144 | 58.568 |
| NO | 30.066 | 21.580 |
| NO2 | 46.066 | 7.910 |
| O | 15.999 | 59.554 |
| O2 | 31.999 | 0.000 |
| HO | 17.009 | 9.317 |

## TABLE B-2
## THERMODYNAMIC DATA FOR SPECIES CONSIDERED IN THE ONE-DIMENSIONAL FLAME CODE

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 4.9760 | 4.9799 | 4.9792 | 4.9762 | 4.9728 | CP | 1 | C |
| 4.9701 | 4.9689 | 4.9694 | 4.9713 | 4.9736 | CP | 2 | C |
| 4.9688 | 4.9661 | 4.9656 | 4.9669 | 4.9702 | CP | 3 | C |
| 4.9752 | 4.9817 | 4.9898 | 4.9993 | 5.0101 | CP | 4 | C |
| 5.0221 | 5.0352 | 5.0492 | 5.0641 | 5.0798 | CP | 5 | C |
| 5.0962 | 5.1131 | 5.1305 | 5.1483 | 5.1665 | CP | 6 | C |
| 5.1848 | 5.2032 | 5.2217 | 5.2401 | 5.2584 | CP | 7 | C |
| 5.2765 | 5.2943 | 5.3117 | 5.3286 | 5.3450 | CP | 8 | C |
| 5.3608 | 5.3759 | 5.3902 | 5.4038 | 5.4164 | CP | 9 | C |
| 5.4281 | 5.4387 | 5.4483 | 5.4567 | 5.4639 | CP | 10 | C |
| -0.9866 | -0.4888 | 0.0092 | 0.5070 | 1.0044 | H | 1 | C |
| 1.5016 | 1.9985 | 2.4954 | 2.9924 | 3.4897 | H | 2 | C |
| 3.9868 | 4.4835 | 4.9801 | 5.4767 | 5.9735 | H | 3 | C |
| 6.4708 | 6.9686 | 7.4672 | 7.9666 | 8.4671 | H | 4 | C |
| 8.9687 | 9.4716 | 9.9758 | 10.4814 | 10.9886 | H | 5 | C |
| 11.4974 | 12.0079 | 12.5200 | 13.0340 | 13.5497 | H | 6 | C |
| 14.0673 | 14.5867 | 15.1079 | 15.6310 | 16.1560 | H | 7 | C |
| 16.6827 | 17.2112 | 17.7415 | 18.2736 | 18.8072 | H | 8 | C |
| 19.3425 | 19.8794 | 20.4177 | 20.9574 | 21.4984 | H | 9 | C |
| 22.0406 | 22.5840 | 23.1284 | 23.6736 | 24.2197 | H | 10 | C |
| 42.1880 | 38.2164 | 37.7610 | 37.9563 | 38.3249 | F | 1 | C |
| 38.7375 | 39.1512 | 39.5505 | 39.9302 | 40.2894 | F | 2 | C |
| 40.6285 | 40.9488 | 41.2517 | 41.5386 | 41.8110 | F | 3 | C |
| 42.0700 | 42.3169 | 42.5526 | 42.7781 | 42.9942 | F | 4 | C |
| 43.2017 | 43.4012 | 43.5933 | 43.7785 | 43.9573 | F | 5 | C |
| 44.1303 | 44.2976 | 44.4598 | 44.6171 | 44.7699 | F | 6 | C |
| 44.9183 | 45.0627 | 45.2033 | 45.3402 | 45.4738 | F | 7 | C |
| 45.6041 | 45.7313 | 45.8556 | 45.9771 | 46.0959 | F | 8 | C |
| 46.2122 | 46.3261 | 46.4376 | 46.5469 | 46.6541 | F | 9 | C |
| 46.7593 | 46.8625 | 46.9638 | 47.0633 | 47.1610 | F | 10 | C |

```
  7.1711     8.1146     8.9199     9.6107    10.2065  CP   1    C2H
 10.7234    11.1733    11.5641    11.9001    12.1814  CP   2    C2H
 12.4276    12.6605    12.8811    13.0900    13.2879  CP   3    C2H
 13.4754    13.6533    13.8221    13.9825    14.1348  CP   4    C2H
 14.2796    14.4174    14.5486    14.6736    14.7927  CP   5    C2H
 14.9063    15.0146    15.1179    15.2165    15.3104  CP   6    C2H
 15.3998    15.4849    15.5657    15.6422    15.7145  CP   7    C2H
 15.7825    15.8462    15.9054    15.9601    16.0099  CP   8    C2H
 16.0549    16.0946    16.1289    16.1573    16.1797  CP   9    C2H
 16.1955    16.2044    16.2059    16.1995    16.1847  CP  10    C2H
 -1.6018    -0.8363     0.0165     0.9439     1.9355  H    1    C2H
  2.9826     4.0779     5.2153     6.3889     7.5935  H    2    C2H
  8.8240    10.0785    11.3557    12.6544    13.9733  H    3    C2H
 15.3116    16.6681    18.0419    19.4322    20.8382  H    4    C2H
 22.2590    23.6939    25.1422    26.6034    28.0767  H    5    C2H
 29.5617    31.0578    32.5645    34.0813    35.6076  H    6    C2H
 37.1432    38.6875    40.2400    41.8004    43.3683  H    7    C2H
 44.9432    46.5247    48.1123    49.7056    51.3041  H    8    C2H
 52.9074    54.5149    56.1252    57.7405    59.3574  H    9    C2H
 60.9762    62.5963    64.2169    65.8372    67.4565  H   10    C2H
 56.9197    50.3516    49.5619    49.9203    50.6193  F    1    C2H
 51.4269    52.2599    53.0845    53.8868    54.6610  F    2    C2H
 55.4053    56.1197    56.8055    57.4642    58.0974  F    3    C2H
 58.7068    59.2941    59.8608    60.4083    60.9378  F    4    C2H
 61.4505    61.9476    62.4299    62.8984    63.3539  F    5    C2H
 63.7971    64.2287    64.6494    65.0597    65.4601  F    6    C2H
 65.8511    66.2332    66.6068    66.9724    67.3301  F    7    C2H
 67.6805    68.0238    68.3603    68.6903    69.0140  F    8    C2H
 69.3317    69.6435    69.9498    70.2507    70.5464  F    9    C2H
 70.8370    71.1228    71.4038    71.6802    71.9522  F   10    C2H
```

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 6.7158 | 8.8912 | 10.6218 | 11.9930 | 13.0810 | CP | 1 | C2H2 |
| 13.9532 | 14.6675 | 15.2730 | 15.8094 | 16.3074 | CP | 2 | C2H2 |
| 16.7737 | 17.2009 | 17.5917 | 17.9486 | 18.2744 | CP | 3 | C2H2 |
| 18.5713 | 18.8417 | 19.0878 | 19.3117 | 19.5155 | CP | 4 | C2H2 |
| 19.7011 | 19.8703 | 20.0247 | 20.1660 | 20.2957 | CP | 5 | C2H2 |
| 20.4152 | 20.5258 | 20.6287 | 20.7249 | 20.8155 | CP | 6 | C2H2 |
| 20.9013 | 20.9831 | 21.0616 | 21.1374 | 21.2109 | CP | 7 | C2H2 |
| 21.2825 | 21.3526 | 21.4211 | 21.4883 | 21.5540 | CP | 8 | C2H2 |
| 21.6181 | 21.6804 | 21.7406 | 21.7981 | 21.8524 | CP | 9 | C2H2 |
| 21.9028 | 21.9487 | 21.9891 | 22.0230 | 22.0494 | CP | 10 | C2H2 |
| -1.7438 | -0.9594 | 0.0196 | 1.1530 | 2.4088 | H | 1 | C2H2 |
| 3.7620 | 5.1942 | 6.6919 | 8.2465 | 9.8525 | H | 2 | C2H2 |
| 11.5069 | 13.2060 | 14.9459 | 16.7232 | 18.5346 | H | 3 | C2H2 |
| 20.3771 | 22.2480 | 24.1446 | 26.0648 | 28.0063 | H | 4 | C2H2 |
| 29.9673 | 31.9460 | 33.9408 | 35.9505 | 37.9737 | H | 5 | C2H2 |
| 40.0093 | 42.0564 | 44.1142 | 46.1819 | 48.2590 | H | 6 | C2H2 |
| 50.3449 | 52.4391 | 54.5414 | 56.6513 | 58.7688 | H | 7 | C2H2 |
| 60.8935 | 63.0252 | 65.1639 | 67.3094 | 69.4615 | H | 8 | C2H2 |
| 71.6202 | 73.7851 | 75.9562 | 78.1331 | 80.3157 | H | 9 | C2H2 |
| 82.5035 | 84.6961 | 86.8930 | 89.0937 | 91.2974 | H | 10 | C2H2 |
| 56.2230 | 48.9323 | 48.0159 | 48.4499 | 49.3125 | F | 1 | C2H2 |
| 50.3248 | 51.3809 | 52.4353 | 53.4678 | 54.4698 | F | 2 | C2H2 |
| 55.4379 | 56.3719 | 57.2725 | 58.1411 | 58.9795 | F | 3 | C2H2 |
| 59.7892 | 60.5720 | 61.3294 | 62.0629 | 62.7739 | F | 4 | C2H2 |
| 63.4636 | 64.1333 | 64.7840 | 65.4168 | 66.0326 | F | 5 | C2H2 |
| 66.6323 | 67.2166 | 67.7863 | 68.3422 | 68.8848 | F | 6 | C2H2 |
| 69.4148 | 69.9327 | 70.4392 | 70.9346 | 71.4194 | F | 7 | C2H2 |
| 71.8942 | 72.3593 | 72.8151 | 73.2620 | 73.7003 | F | 8 | C2H2 |
| 74.1303 | 74.5525 | 74.9670 | 75.3742 | 75.7742 | F | 9 | C2H2 |
| 76.1675 | 76.5541 | 76.9344 | 77.3085 | 77.6766 | F | 10 | C2H2 |

```
  6.3904     7.9589     9.5681    11.1879    12.7828  CP  1    C2H3
 14.3118    15.7278    16.9785    18.0058    18.7458  CP  2    C2H3
 19.3057    19.8379    20.3418    20.8173    21.2640  CP  3    C2H3
 21.6820    22.0712    22.4319    22.7643    23.0687  CP  4    C2H3
 23.3458    23.5959    23.8200    24.0188    24.1933  CP  5    C2H3
 24.3445    24.4737    24.5820    24.6709    24.7420  CP  6    C2H3
 24.7968    24.8370    24.8646    24.8815    24.8898  CP  7    C2H3
 24.8917    24.8895    24.8856    24.8825    24.8830  CP  8    C2H3
 24.8897    24.9055    24.9335    24.9767    25.0383  CP  9    C2H3
 25.1217    25.2303    25.3677    25.5376    25.7436  CP 10    C2H3
 -1.5755    -0.8585     0.0177     1.0555     2.2544  H   1    C2H3
  3.6099     5.1130     6.7499     8.5013    10.3415  H   2    C2H3
 12.2443    14.2017    16.2110    18.2692    20.3735  H   3    C2H3
 22.5210    24.7089    26.9343    29.1943    31.4862  H   4    C2H3
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 71.5126    72.2693    73.0069    73.7261    74.4279  F   5    C2H3
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 78.3095    78.9071    79.4921    80.0648    80.6257  F   7    C2H3
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| 8.0093 | 8.2181 | 8.4105 | 8.5872 | 8.7491 | CP | 3 | CH |
| 8.8970 | 9.0317 | 9.1539 | 9.2644 | 9.3640 | CP | 4 | CH |
| 9.4533 | 9.5331 | 9.6039 | 9.6666 | 9.7217 | CP | 5 | CH |
| 9.7698 | 9.8116 | 9.8477 | 9.8785 | 9.9047 | CP | 6 | CH |
| 9.9269 | 9.9454 | 9.9608 | 9.9736 | 9.9842 | CP | 7 | CH |
| 9.9931 | 10.0007 | 10.0074 | 10.0136 | 10.0196 | CP | 8 | CH |
| 10.0259 | 10.0326 | 10.0402 | 10.0489 | 10.0591 | CP | 9 | CH |
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| 34.4417 | 35.4446 | 36.4483 | 37.4527 | 38.4581 | H | 9 | CH |
| 39.4646 | 40.4723 | 41.4815 | 42.4925 | 43.5053 | H | 10 | CH |
| 49.8292 | 44.3506 | 43.7174 | 43.9908 | 44.5087 | F | 1 | CH |
| 45.0904 | 45.6762 | 46.2449 | 46.7898 | 47.3098 | F | 2 | CH |
| 47.8061 | 48.2805 | 48.7346 | 49.1700 | 49.5883 | F | 3 | CH |
| 49.9908 | 50.3786 | 50.7529 | 51.1146 | 51.4644 | F | 4 | CH |
| 51.8033 | 52.1318 | 52.4506 | 52.7602 | 53.0612 | F | 5 | CH |
| 53.3540 | 53.6390 | 53.9166 | 54.1872 | 54.4512 | F | 6 | CH |
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| 32.5595 | 33.8858 | 35.2147 | 36.5459 | 37.8796 | H | 7 | CH2 |
| 39.2162 | 40.5560 | 41.8999 | 43.2487 | 44.6035 | H | 8 | CH2 |
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| 52.9465 | 54.3927 | 55.8620 | 57.3578 | 58.8838 | H | 10 | CH2 |
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| 57.1381 | 57.5745 | 57.9981 | 58.4097 | 58.8099 | F | 5 | CH2 |
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 23.5030   23.7175   23.9055   24.0695   24.2117  CP  5   CH30
 24.3345   24.4399   24.5300   24.6066   24.6717  CP  6   CH30
 24.7270   24.7741   24.8145   24.8497   24.8809  CP  7   CH30
 24.9094   24.9364   24.9629   24.9897   25.0177  CP  8   CH30
 25.0477   25.0802   25.1158   25.1549   25.1978  CP  9   CH30
 25.2448   25.2959   25.3512   25.4105   25.4738  CP 10   CH30
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 11.9937   13.9552   15.9775   18.0549   20.1825  H   3   CH30
 22.3554   24.5692   26.8196   29.1028   31.4153  H   4   CH30
 33.7537   36.1149   38.4963   40.8952   43.3095  H   5   CH30
 45.7369   48.1758   50.6244   53.0813   55.5453  H   6   CH30
 58.0153   60.4905   62.9699   65.4532   67.9397  H   7   CH30
 70.4293   72.9216   75.4166   77.9142   80.4145  H   8   CH30
 82.9178   85.4242   87.9339   90.4474   92.9650  H   9   CH30
 95.4871   98.0141  100.5465  103.0845  105.6287  H  10   CH30
 61.4726   55.3762   54.6035   54.9801   55.7473  F   1   CH30
 56.6738   57.6686   58.6896   59.7147   60.7315  F   2   CH30
 61.7324   62.7128   63.6702   64.6035   65.5125  F   3   CH30
 66.3976   67.2592   68.0981   68.9150   69.7108  F   4   CH30
 70.4861   71.2418   71.9787   72.6975   73.3989  F   5   CH30
 74.0836   74.7523   75.4055   76.0439   76.6680  F   6   CH30
 77.2784   77.8756   78.4600   79.0322   79.5926  F   7   CH30
 80.1416   80.6796   81.2070   81.7243   82.2316  F   8   CH30
 82.7295   83.2183   83.6982   84.1695   84.6326  F   9   CH30
 85.0878   85.5353   85.9753   86.4081   86.8341  F  10   CH30
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 18.0673   18.8112   19.4827   20.0872   20.6299  CP  3   CH4
 21.1158   21.5496   21.9359   22.2789   22.5830  CP  4   CH4
 22.8518   23.0892   23.2985   23.4831   23.6460  CP  5   CH4
 23.7900   23.9177   24.0316   24.1337   24.2262  CP  6   CH4
 24.3107   24.3887   24.4617   24.5306   24.5965  CP  7   CH4
 24.6600   24.7215   24.7813   24.8395   24.8958  CP  8   CH4
 24.9499   25.0011   25.0487   25.0916   25.1285  CP  9   CH4
 25.1581   25.1785   25.1879   25.1842   25.1651  CP 10   CH4
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 31.8002   34.0975   36.4171   38.7563   41.1130  H   5   CH4
 43.4849   45.8704   48.2680   50.6763   53.0944  H   6   CH4
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 92.7048   95.2217   97.7401  100.2588  102.7764  H  10   CH4
 50.7381   45.1817   44.4651   44.8132   45.5161  F   1   CH4
 46.3571   47.2538   48.1713   49.0933   50.0111  F   2   CH4
 50.9187   51.8120   52.6885   53.5469   54.3865  F   3   CH4
 55.2071   56.0089   56.7919   57.5568   58.3037  F   4   CH4
 59.0333   59.7461   60.4425   61.1231   61.7884  F   5   CH4
 62.4389   63.0751   63.6975   64.3065   64.9028  F   6   CH4
 65.4866   66.0584   66.6187   67.1678   67.7061  F   7   CH4
 68.2341   68.7521   69.2603   69.7593   70.2492  F   8   CH4
 70.7304   71.2031   71.6677   72.1245   72.5736  F   9   CH4
 73.0153   73.4499   73.8775   74.2984   74.7127  F  10   CH4
 7.0922    6.9915    6.9730    7.0292    7.1485  CP  1   CN
 7.3155    7.5110    7.7116    7.8902    8.0156  CP  2   CN
 8.1050    8.1976    8.2932    8.3913    8.4916  CP  3   CN
 8.5937    8.6972    8.8019    8.9074    9.0133  CP  4   CN
 9.1193    9.2251    9.3303    9.4347    9.5380  CP  5   CN
 9.6398    9.7399    9.8380    9.9338   10.0270  CP  6   CN
10.1174   10.2046   10.2885   10.3689   10.4454  CP  7   CN
10.5178   10.5859   10.6495   10.7084   10.7623  CP  8   CN
10.8110   10.8545   10.8923   10.9245   10.9508  CP  9   CN
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54.7892   55.1798   55.5554   55.9172   56.2663  F   4   CN
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58.1407   58.4227   58.6974   58.9654   59.2268  F   6   CN
59.4822   59.7318   59.9760   60.2150   60.4490  F   7   CN
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61.7611   61.9661   62.1676   62.3656   62.5604  F   9   CN
62.7520   62.9405   63.1260   63.3087   63.4885  F  10   CN
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 8.0596    8.1609    8.2520    8.3338    8.4069  CP  3   CO
 8.4722    8.5303    8.5819    8.6276    8.6681  CP  4   CO
 8.7039    8.7356    8.7636    8.7884    8.8106  CP  5   CO
 8.8304    8.8482    8.8645    8.8794    8.8934  CP  6   CO
 8.9065    8.9191    8.9313    8.9432    8.9550  CP  7   CO
 8.9668    8.9785    8.9902    9.0019    9.0135  CP  8   CO
 9.0249    9.0360    9.0467    9.0568    9.0660  CP  9   CO
 9.0741    9.0808    9.0858    9.0888    9.0893  CP 10   CO
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 5.9856    6.7967    7.6174    8.4468    9.2839  H   3   CO
10.1279   10.9781   11.8337   12.6943   13.5591  H   4   CO
14.4277   15.2997   16.1747   17.0524   17.9323  H   5   CO
18.8144   19.6983   20.5840   21.4712   22.3598  H   6   CO
23.2498   24.1411   25.0336   25.9274   26.8223  H   7   CO
27.7184   28.6156   29.5141   30.4137   31.3145  H   8   CO
32.2164   33.1194   34.0236   34.9288   35.8349  H   9   CO
36.7419   37.6497   38.5580   39.4668   40.3757  H  10   CO
53.3209   47.8432   47.2107   47.4842   48.0037  F   1   CO
48.5895   49.1816   49.7589   50.3138   50.8445  F   2   CO
51.3510   51.8342   52.2954   52.7362   53.1578  F   3   CO
53.5619   53.9495   54.3220   54.6803   55.0256  F   4   CO
55.3586   55.6801   55.9910   56.2919   56.5833  F   5   CO
56.8659   57.1401   57.4064   57.6653   57.9172  F   6   CO
58.1623   58.4012   58.6339   58.8610   59.0826  F   7   CO
59.2990   59.5104   59.7171   59.9193   60.1171  F   8   CO
60.3108   60.5005   60.6863   60.8685   61.0472  F   9   CO
61.2225   61.3945   61.5634   61.7293   61.8922  F  10   CO
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 14.0607   14.1754   14.2763   14.3648   14.4425  CP  4    CO2
 14.5104   14.5699   14.6222   14.6682   14.7090  CP  5    CO2
 14.7455   14.7785   14.8087   14.8368   14.8634  CP  6    CO2
 14.8890   14.9140   14.9388   14.9636   14.9886  CP  7    CO2
 15.0140   15.0398   15.0658   15.0921   15.1183  CP  8    CO2
 15.1441   15.1693   15.1934   15.2158   15.2359  CP  9    CO2
 15.2530   15.2665   15.2753   15.2786   15.2755  CP 10    CO2
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  9.2990   10.6320   11.9847   13.3549   14.7408  H   3    CO2
 16.1405   17.5524   18.9751   20.4073   21.8477  H   4    CO2
 23.2954   24.7495   26.2092   27.6738   29.1427  H   5    CO2
 30.6154   32.0916   33.5710   35.0533   36.5383  H   6    CO2
 38.0259   39.5161   41.0087   42.5039   44.0015  H   7    CO2
 45.5016   47.0043   48.5096   50.0174   51.5280  H   8    CO2
 53.0411   54.5568   56.0749   57.5954   59.1180  H   9    CO2
 60.6425   62.1685   63.6956   65.2234   66.7511  H  10    CO2
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 57.1461   57.8995   58.6231   59.3183   59.9864  F   3    CO2
 60.6291   61.2479   61.8443   62.4196   62.9753  F   4    CO2
 63.5124   64.0321   64.5354   65.0233   65.4966  F   5    CO2
 65.9561   66.4026   66.8368   67.2592   67.6706  F   6    CO2
 68.0714   68.4621   68.8433   69.2154   69.5788  F   7    CO2
 69.9339   70.2811   70.6207   70.9531   71.2785  F   8    CO2
 71.5973   71.9097   72.2159   72.5163   72.8110  F   9    CO2
 73.1003   73.3843   73.6632   73.9372   74.2065  F  10    CO2
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  4.9675     4.9675     4.9675     4.9675     4.9675  CP  2    H
  4.9675     4.9675     4.9675     4.9675     4.9675  CP  3    H
  4.9675     4.9675     4.9675     4.9675     4.9675  CP  4    H
  4.9675     4.9675     4.9675     4.9675     4.9675  CP  5    H
  4.9675     4.9675     4.9675     4.9675     4.9675  CP  6    H
  4.9675     4.9675     4.9675     4.9675     4.9675  CP  7    H
  4.9675     4.9675     4.9675     4.9675     4.9675  CP  8    H
  4.9675     4.9675     4.9675     4.9675     4.9675  CP  9    H
  4.9675     4.9675     4.9675     4.9675     4.9675  CP 10    H
 -0.9843    -0.4876     0.0092     0.5059     1.0027  H   1    H
  1.4994     1.9962     2.4929     2.9897     3.4864  H   2    H
  3.9832     4.4799     4.9767     5.4734     5.9702  H   3    H
  6.4669     6.9637     7.4604     7.9572     8.4539  H   4    H
  8.9507     9.4474     9.9442    10.4409    10.9377  H   5    H
 11.4344    11.9312    12.4279    12.9247    13.4214  H   6    H
 13.9182    14.4149    14.9117    15.4084    15.9052  H   7    H
 16.4019    16.8987    17.3954    17.8922    18.3889  H   8    H
 18.8857    19.3824    19.8792    20.3759    20.8727  H   9    H
 21.3694    21.8662    22.3629    22.8597    23.3564  H  10    H
 31.8050    27.8429    27.3887    27.5835    27.9514  F   1    H
 28.3634    28.7765    29.1754    29.5548    29.9136  F   2    H
 30.2524    30.5724    30.8751    31.1618    31.4340  F   3    H
 31.6929    31.9396    32.1752    32.4004    32.6163  F   4    H
 32.8234    33.0224    33.2139    33.3985    33.5766  F   5    H
 33.7487    33.9150    34.0761    34.2322    34.3836  F   6    H
 34.5305    34.6733    34.8121    34.9472    35.0788  F   7    H
 35.2070    35.3320    35.4539    35.5729    35.6892  F   8    H
 35.8028    35.9139    36.0226    36.1290    36.2331  F   9    H
 36.3352    36.4352    36.5332    36.6293    36.7236  F  10    H
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|  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|
| 6.7010 | 6.8163 | 6.9011 | 6.9591 | 6.9963 | CP | 1 | H2 |
| 7.0202 | 7.0406 | 7.0693 | 7.1198 | 7.2078 | CP | 2 | H2 |
| 7.3188 | 7.4268 | 7.5318 | 7.6337 | 7.7326 | CP | 3 | H2 |
| 7.8285 | 7.9213 | 8.0111 | 8.0980 | 8.1818 | CP | 4 | H2 |
| 8.2627 | 8.3408 | 8.4160 | 8.4884 | 8.5581 | CP | 5 | H2 |
| 8.6252 | 8.6897 | 8.7518 | 8.8116 | 8.8690 | CP | 6 | H2 |
| 8.9243 | 8.9776 | 9.0290 | 9.0787 | 9.1267 | CP | 7 | H2 |
| 9.1733 | 9.2185 | 9.2626 | 9.3058 | 9.3481 | CP | 8 | H2 |
| 9.3898 | 9.4312 | 9.4723 | 9.5134 | 9.5548 | CP | 9 | H2 |
| 9.5966 | 9.6391 | 9.6826 | 9.7272 | 9.7732 | CP | 10 | H2 |
| -1.3495 | -0.6733 | 0.0128 | 0.7060 | 1.4039 | H | 1 | H2 |
| 2.1048 | 2.8078 | 3.5132 | 4.2224 | 4.9384 | H | 2 | H2 |
| 5.6648 | 6.4021 | 7.1500 | 7.9083 | 8.6767 | H | 3 | H2 |
| 9.4548 | 10.2423 | 11.0389 | 11.8444 | 12.6584 | H | 4 | H2 |
| 13.4807 | 14.3109 | 15.1487 | 15.9940 | 16.8463 | H | 5 | H2 |
| 17.7055 | 18.5713 | 19.4434 | 20.3216 | 21.2056 | H | 6 | H2 |
| 22.0953 | 22.9904 | 23.8908 | 24.7962 | 25.7064 | H | 7 | H2 |
| 26.6214 | 27.5410 | 28.4651 | 29.3935 | 30.3262 | H | 8 | H2 |
| 31.2631 | 32.2042 | 33.1494 | 34.0987 | 35.0521 | H | 9 | H2 |
| 36.0096 | 36.9714 | 37.9375 | 38.9080 | 39.8830 | H | 10 | H2 |
| 37.2846 | 31.8385 | 31.2100 | 31.4815 | 31.9958 | F | 1 | H2 |
| 32.5734 | 33.1539 | 33.7155 | 34.2507 | 34.7581 | F | 2 | H2 |
| 35.2390 | 35.6952 | 36.1288 | 36.5420 | 36.9364 | F | 3 | H2 |
| 37.3137 | 37.6755 | 38.0229 | 38.3573 | 38.6795 | F | 4 | H2 |
| 38.9905 | 39.2911 | 39.5821 | 39.8640 | 40.1376 | F | 5 | H2 |
| 40.4033 | 40.6616 | 40.9129 | 41.1577 | 41.3963 | F | 6 | H2 |
| 41.6291 | 41.8562 | 42.0782 | 42.2951 | 42.5072 | F | 7 | H2 |
| 42.7149 | 42.9181 | 43.1173 | 43.3125 | 43.5038 | F | 8 | H2 |
| 43.6916 | 43.8758 | 44.0568 | 44.2344 | 44.4091 | F | 9 | H2 |
| 44.5807 | 44.7494 | 44.9154 | 45.0788 | 45.2396 | F | 10 | H2 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 7.3072 | 7.7083 | 7.9982 | 8.2300 | 8.4449 | CP | 1 | H2O |
| 8.6723 | 8.9294 | 9.2217 | 9.5427 | 9.8736 | CP | 2 | H2O |
| 10.1897 | 10.4850 | 10.7606 | 11.0176 | 11.2569 | CP | 3 | H2O |
| 11.4795 | 11.6865 | 11.8787 | 12.0570 | 12.2224 | CP | 4 | H2O |
| 12.3755 | 12.5174 | 12.6486 | 12.7701 | 12.8824 | CP | 5 | H2O |
| 12.9863 | 13.0825 | 13.1714 | 13.2539 | 13.3303 | CP | 6 | H2O |
| 13.4013 | 13.4673 | 13.5289 | 13.5864 | 13.6402 | CP | 7 | H2O |
| 13.6908 | 13.7386 | 13.7837 | 13.8265 | 13.8673 | CP | 8 | H2O |
| 13.9063 | 13.9437 | 13.9796 | 14.0143 | 14.0477 | CP | 9 | H2O |
| 14.0800 | 14.1112 | 14.1414 | 14.1705 | 14.1984 | CP | 10 | H2O |
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| 2.5159 | 3.3957 | 4.3030 | 5.2410 | 6.2119 | H | 2 | H2O |
| 7.2152 | 8.2491 | 9.3116 | 10.4006 | 11.5145 | H | 3 | H2O |
| 12.6514 | 13.8099 | 14.9882 | 16.1851 | 17.3992 | H | 4 | H2O |
| 18.6292 | 19.8739 | 21.1323 | 22.4033 | 23.6860 | H | 5 | H2O |
| 24.9795 | 26.2830 | 27.5958 | 28.9171 | 30.2464 | H | 6 | H2O |
| 31.5830 | 32.9265 | 34.2763 | 35.6321 | 36.9935 | H | 7 | H2O |
| 38.3600 | 39.7315 | 41.1077 | 42.4882 | 43.8729 | H | 8 | H2O |
| 45.2616 | 46.6541 | 48.0503 | 49.4500 | 50.8531 | H | 9 | H2O |
| 52.2595 | 53.6691 | 55.0817 | 56.4973 | 57.9158 | H | 10 | H2O |
| 52.0016 | 45.8221 | 45.0997 | 45.4163 | 46.0217 | F | 1 | H2O |
| 46.7084 | 47.4063 | 48.0896 | 48.7495 | 49.3835 | F | 2 | H2O |
| 49.9922 | 50.5766 | 51.1384 | 51.6791 | 52.2002 | F | 3 | H2O |
| 52.7030 | 53.1890 | 53.6591 | 54.1145 | 54.5561 | F | 4 | H2O |
| 54.9847 | 55.4012 | 55.8062 | 56.2003 | 56.5843 | F | 5 | H2O |
| 56.9585 | 57.3235 | 57.6797 | 58.0276 | 58.3675 | F | 6 | H2O |
| 58.6998 | 59.0249 | 59.3430 | 59.6545 | 59.9596 | F | 7 | H2O |
| 60.2585 | 60.5516 | 60.8391 | 61.1211 | 61.3978 | F | 8 | H2O |
| 61.6695 | 61.9364 | 62.1986 | 62.4562 | 62.7094 | F | 9 | H2O |
| 62.9585 | 63.2034 | 63.4444 | 63.6816 | 63.9151 | F | 10 | H2O |

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 18.0272   18.1630   18.2853   18.3953   18.4943  CP   5    H2O2
 18.5833   18.6634   18.7357   18.8010   18.8602  CP   6    H2O2
 18.9140   18.9633   19.0086   19.0505   19.0896  CP   7    H2O2
 19.1263   19.1609   19.1938   19.2252   19.2553  CP   8    H2O2
 19.2842   19.3119   19.3384   19.3635   19.3872  CP   9    H2O2
 19.4092   19.4292   19.4467   19.4614   19.4728  CP  10    H2O2
 -1.8310   -0.9657    0.0192    1.1133    2.3038  H    1    H2O2
  3.5777    4.9217    6.3247    7.7779    9.2766  H    2    H2O2
 10.8174   12.3953   14.0072   15.6503   17.3218  H    3    H2O2
 19.0192   20.7403   22.4828   24.2446   26.0241  H    4    H2O2
 27.8194   29.6290   31.4515   33.2857   35.1302  H    5    H2O2
 36.9842   38.8466   40.7166   42.5935   44.4766  H    6    H2O2
 46.3654   48.2593   50.1579   52.0609   53.9679  H    7    H2O2
 55.8787   57.7931   59.7108   61.6318   63.5558  H    8    H2O2
 65.4828   67.4126   69.3451   71.2803   73.2178  H    9    H2O2
 75.1576   77.0996   79.0434   80.9888   82.9356  H   10    H2O2
 64.1021   56.5691   55.6544   56.0756   56.9040  F    1    H2O2
 57.8692   58.8716   59.8694   60.8442   61.7883  F    2    H2O2
 62.6992   63.5765   64.4212   65.2347   66.0187  F    3    H2O2
 66.7750   67.5051   68.2108   68.8934   69.5544  F    4    H2O2
 70.1951   70.8165   71.4197   72.0059   72.5758  F    5    H2O2
 73.1303   73.6702   74.1963   74.7091   75.2094  F    6    H2O2
 75.6977   76.1745   76.6404   77.0959   77.5413  F    7    H2O2
 77.9771   78.4037   78.8215   79.2309   79.6321  F    8    H2O2
 80.0254   80.4112   80.7898   81.1614   81.5263  F    9    H2O2
 81.8846   82.2367   82.5827   82.9229   83.2574  F   10    H2O2
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  6.4692     7.6630     8.6034     9.3529     9.9636  CP  1    CHN
 10.4767    10.9230    11.3226    11.6850    12.0090  CP  2    CHN
 12.2972    12.5596    12.7980    13.0142    13.2098  CP  3    CHN
 13.3865    13.5459    13.6894    13.8184    13.9343  CP  4    CHN
 14.0383    14.1317    14.2156    14.2909    14.3588  CP  5    CHN
 14.4202    14.4758    14.5265    14.5730    14.6158  CP  6    CHN
 14.6556    14.6929    14.7281    14.7616    14.7935  CP  7    CHN
 14.8243    14.8539    14.8824    14.9099    14.9363  CP  8    CHN
 14.9615    14.9852    15.0072    15.0271    15.0445  CP  9    CHN
 15.0589    15.0697    15.0764    15.0781    15.0743  CP 10    CHN
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  8.6389     9.8819    11.1500    12.4408    13.7522  H   3    CHN
 15.0821    16.4289    17.7908    19.1663    20.5540  H   4    CHN
 21.9528    23.3613    24.7788    26.2042    27.6367  H   5    CHN
 29.0757    30.5206    31.9707    33.4257    34.8852  H   6    CHN
 36.3488    37.8162    39.2873    40.7618    42.2396  H   7    CHN
 43.7205    45.2044    46.6912    48.1808    49.6732  H   8    CHN
 51.1681    52.6654    54.1651    55.6668    57.1704  H   9    CHN
 58.6756    60.1820    61.6894    63.1972    64.7048  H  10    CHN
 55.1923    48.9727    48.2157    48.5627    49.2414  F   1    CHN
 50.0274    50.8390    51.6431    52.4261    53.1824  F   2    CHN
 53.9106    54.6106    55.2835    55.9306    56.5534  F   3    CHN
 57.1535    57.7322    58.2909    58.8308    59.3531  F   4    CHN
 59.8588    60.3490    60.8245    61.2861    61.7346  F   5    CHN
 62.1707    62.5950    63.0082    63.4108    63.8033  F   6    CHN
 64.1861    64.5599    64.9249    65.2815    65.6302  F   7    CHN
 65.9713    66.3050    66.6318    66.9518    67.2654  F   8    CHN
 67.5728    67.8743    68.1700    68.4602    68.7451  F   9    CHN
 69.0249    69.2998    69.5699    69.8353    70.0963  F  10    CHN
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 11.7745    12.0033    12.2085    12.3920    12.5557  CP  3    CHO
 12.7013    12.8305    12.9449    13.0461    13.1353  CP  4    CHO
 13.2141    13.2837    13.3452    13.3998    13.4484  CP  5    CHO
 13.4921    13.5318    13.5680    13.6017    13.6333  CP  6    CHO
 13.6635    13.6926    13.7211    13.7493    13.7772  CP  7    CHO
 13.8052    13.8331    13.8611    13.8889    13.9163  CP  8    CHO
 13.9431    13.9689    13.9933    14.0157    14.0356  CP  9    CHO
 14.0522    14.0647    14.0723    14.0741    14.0691  CP 10    CHO
 -1.5025    -0.7789     0.0152     0.8670     1.7699  H   1    CHO
  2.7220     3.7231     4.7731     5.8696     7.0057  H   2    CHO
  8.1707     9.3598    10.5705    11.8007    13.0483  H   3    CHO
 14.3113    15.5880    16.8769    18.1765    19.4857  H   4    CHO
 20.8032    22.1282    23.4597    24.7970    26.1395  H   5    CHO
 27.4865    28.8378    30.1928    31.5513    32.9130  H   6    CHO
 34.2779    35.6457    37.0164    38.3899    39.7663  H   7    CHO
 41.1454    42.5273    43.9120    45.2995    46.6898  H   8    CHO
 48.0827    49.4783    50.8765    52.2769    53.6795  H   9    CHO
 55.0840    56.4898    57.8967    59.3041    60.7113  H  10    CHO
 60.5392    54.3928    53.6590    53.9889    54.6293  F   1    CHO
 55.3670    56.1272    56.8809    57.6165    58.3292  F   2    CHO
 59.0172    59.6798    60.3174    60.9311    61.5220  F   3    CHO
 62.0914    62.6405    63.1705    63.6826    64.1779  F   4    CHO
 64.6572    65.1216    65.5719    66.0088    66.4331  F   5    CHO
 66.8455    67.2465    67.6368    68.0169    68.3873  F   6    CHO
 68.7485    69.1008    69.4448    69.7808    70.1091  F   7    CHO
 70.4301    70.7442    71.0515    71.3525    71.6473  F   8    CHO
 71.9362    72.2194    72.4972    72.7698    73.0373  F   9    CHO
 73.3000    73.5580    73.8115    74.0607    74.3056  F  10    CHO
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| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 8.6553 | 9.9308 | 11.1350 | 12.2427 | 13.2352 | CP | 1 | HNCO |
| 14.1003 | 14.8323 | 15.4318 | 15.9063 | 16.2694 | CP | 2 | HNCO |
| 16.5739 | 16.8602 | 17.1280 | 17.3772 | 17.6079 | CP | 3 | HNCO |
| 17.8201 | 18.0140 | 18.1901 | 18.3486 | 18.4903 | CP | 4 | HNCO |
| 18.6157 | 18.7256 | 18.8209 | 18.9025 | 18.9716 | CP | 5 | HNCO |
| 19.0293 | 19.0769 | 19.1160 | 19.1479 | 19.1743 | CP | 6 | HNCO |
| 19.1970 | 19.2178 | 19.2387 | 19.2617 | 19.2890 | CP | 7 | HNCO |
| 19.3229 | 19.3658 | 19.4201 | 19.4885 | 19.5737 | CP | 8 | HNCO |
| 19.6785 | 19.8059 | 19.9589 | 20.1406 | 20.3543 | CP | 9 | HNCO |
| 20.6034 | 20.8913 | 21.2216 | 21.5980 | 22.0243 | CP | 10 | HNCO |
| -1.9632 | -1.0334 | 0.0206 | 1.1904 | 2.4653 | H | 1 | HNCO |
| 3.8331 | 5.2809 | 6.7952 | 8.3631 | 9.9727 | H | 2 | HNCO |
| 11.6150 | 13.2869 | 14.9865 | 16.7119 | 18.4613 | H | 3 | HNCO |
| 20.2328 | 22.0247 | 23.8350 | 25.6621 | 27.5042 | H | 4 | HNCO |
| 29.3596 | 31.2268 | 33.1043 | 34.9906 | 36.8844 | H | 5 | HNCO |
| 38.7845 | 40.6899 | 42.5996 | 44.5128 | 46.4290 | H | 6 | HNCO |
| 48.3476 | 50.2683 | 52.1912 | 54.1161 | 56.0436 | H | 7 | HNCO |
| 57.9742 | 59.9085 | 61.8477 | 63.7930 | 65.7460 | H | 8 | HNCO |
| 67.7084 | 69.6824 | 71.6704 | 73.6752 | 75.6996 | H | 9 | HNCO |
| 77.7472 | 79.8216 | 81.9269 | 84.0674 | 86.2481 | H | 10 | HNCO |
| 66.1056 | 58.0347 | 57.0561 | 57.5065 | 58.3926 | F | 1 | HNCO |
| 59.4261 | 60.5008 | 61.5721 | 62.6199 | 63.6351 | F | 2 | HNCO |
| 64.6138 | 65.5550 | 66.4596 | 67.3291 | 68.1656 | F | 3 | HNCO |
| 68.9708 | 69.7469 | 70.4956 | 71.2187 | 71.9178 | F | 4 | HNCO |
| 72.5944 | 73.2498 | 73.8852 | 74.5017 | 75.1005 | F | 5 | HNCO |
| 75.6823 | 76.2482 | 76.7989 | 77.3352 | 77.8577 | F | 6 | HNCO |
| 78.3671 | 78.8641 | 79.3491 | 79.8228 | 80.2855 | F | 7 | HNCO |
| 80.7379 | 81.1804 | 81.6133 | 82.0371 | 82.4522 | F | 8 | HNCO |
| 82.8591 | 83.2579 | 83.6492 | 84.0333 | 84.4104 | F | 9 | HNCO |
| 84.7810 | 85.1454 | 85.5038 | 85.8567 | 86.2042 | F | 10 | HNCO |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 6.6792 | 7.5582 | 8.2554 | 8.8385 | 9.3575 | CP | 1 | HNO |
| 9.8442 | 10.3128 | 10.7595 | 11.1625 | 11.4822 | CP | 2 | HNO |
| 11.7296 | 11.9522 | 12.1518 | 12.3303 | 12.4894 | CP | 3 | HNO |
| 12.6307 | 12.7558 | 12.8661 | 12.9632 | 13.0482 | CP | 4 | HNO |
| 13.1227 | 13.1876 | 13.2441 | 13.2934 | 13.3364 | CP | 5 | HNO |
| 13.3739 | 13.4069 | 13.4360 | 13.4621 | 13.4856 | CP | 6 | HNO |
| 13.5072 | 13.5272 | 13.5462 | 13.5644 | 13.5820 | CP | 7 | HNO |
| 13.5993 | 13.6164 | 13.6332 | 13.6497 | 13.6659 | CP | 8 | HNO |
| 13.6814 | 13.6962 | 13.7097 | 13.7217 | 13.7316 | CP | 9 | HNO |
| 13.7389 | 13.7429 | 13.7429 | 13.7383 | 13.7280 | CP | 10 | HNO |
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| 14.3047 | 15.5742 | 16.8554 | 18.1470 | 19.4476 | H | 4 | HNO |
| 20.7563 | 22.0718 | 23.3935 | 24.7204 | 26.0520 | H | 5 | HNO |
| 27.3875 | 28.7266 | 30.0688 | 31.4137 | 32.7611 | H | 6 | HNO |
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| 40.8881 | 42.2489 | 43.6114 | 44.9755 | 46.3413 | H | 8 | HNO |
| 47.7087 | 49.0776 | 50.4479 | 51.8194 | 53.1921 | H | 9 | HNO |
| 54.5657 | 55.9398 | 57.3141 | 58.6882 | 60.0616 | H | 10 | HNO |
| 59.5628 | 53.4545 | 52.7218 | 53.0529 | 53.6967 | F | 1 | HNO |
| 54.4393 | 55.2048 | 55.9636 | 56.7034 | 57.4193 | F | 2 | HNO |
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| 61.1869 | 61.7356 | 62.2651 | 62.7764 | 63.2708 | F | 4 | HNO |
| 63.7491 | 64.2124 | 64.6615 | 65.0971 | 65.5200 | F | 5 | HNO |
| 65.9310 | 66.3305 | 66.7193 | 67.0978 | 67.4665 | F | 6 | HNO |
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| 70.9938 | 71.2748 | 71.5503 | 71.8205 | 72.0857 | F | 9 | HNO |
| 72.3459 | 72.6015 | 72.8525 | 73.0991 | 73.3414 | F | 10 | HNO |

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  9.9686   10.3986   10.7797   11.1108   11.3874  CP  2   HO2
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 12.6276   12.7921   12.9460   13.0896   13.2236  CP  4   HO2
 13.3483   13.4643   13.5719   13.6716   13.7638  CP  5   HO2
 13.8488   13.9272   13.9991   14.0651   14.1254  CP  6   HO2
 14.1804   14.2304   14.2757   14.3165   14.3532  CP  7   HO2
 14.3860   14.4151   14.4408   14.4634   14.4830  CP  8   HO2
 14.4997   14.5139   14.5257   14.5351   14.5424  CP  9   HO2
 14.5477   14.5511   14.5526   14.5525   14.5506  CP 10   HO2
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 14.3014   15.5725   16.8594   18.1613   19.4770  H   4   HO2
 20.8057   22.1464   23.4983   24.8605   26.2324  H   5   HO2
 27.6130   29.0019   30.3983   31.8015   33.2111  H   6   HO2
 34.6264   36.0470   37.4724   38.9020   40.3355  H   7   HO2
 41.7725   43.2126   44.6554   46.1006   47.5480  H   8   HO2
 48.9971   50.4478   51.8998   53.3529   54.8068  H   9   HO2
 56.2613   57.7163   59.1715   60.6267   62.0819  H  10   HO2
 61.6429   55.4654   54.7258   55.0602   55.7114  F   1   HO2
 56.4632   57.2382   58.0055   58.7523   59.4733  F   2   HO2
 60.1669   60.8330   61.4727   62.0873   62.6784  F   3   HO2
 63.2476   63.7962   64.3257   64.8373   65.3322  F   4   HO2
 65.8115   66.2761   66.7269   67.1648   67.5904  F   5   HO2
 68.0044   68.4075   68.8003   69.1832   69.5567  F   6   HO2
 69.9213   70.2775   70.6255   70.9658   71.2986  F   7   HO2
 71.6244   71.9434   72.2558   72.5620   72.8621  F   8   HO2
 73.1564   73.4451   73.7284   74.0065   74.2796  F   9   HO2
 74.5479   74.8115   75.0705   75.3252   75.5756  F  10   HO2
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 15.4649   15.7540   16.0248   16.2773   16.5113  CP  3    HOCN
 16.7270   16.9247   17.1045   17.2670   17.4127  CP  4    HOCN
 17.5422   17.6562   17.7556   17.8413   17.9144  CP  5    HOCN
 17.9761   18.0277   18.0705   18.1059   18.1357  CP  6    HOCN
 18.1615   18.1851   18.2085   18.2336   18.2625  CP  7    HOCN
 18.2976   18.3411   18.3956   18.4635   18.5475  CP  8    HOCN
 18.6504   18.7750   18.9244   19.1017   19.3100  CP  9    HOCN
 19.5526   19.8329   20.1545   20.5210   20.9361  CP 10    HOCN
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 27.4554   29.2154   30.9862   32.7661   34.5540  H   5    HOCN
 36.3486   38.1489   39.9539   41.7627   43.5749  H   6    HOCN
 45.3897   47.2071   49.0268   50.8488   52.6736  H   7    HOCN
 54.5015   56.3334   58.1701   60.0130   61.8634  H   8    HOCN
 63.7231   65.5942   67.4789   69.3800   71.3003  H   9    HOCN
 73.2431   75.2121   77.2111   79.2445   81.3169  H  10    HOCN
 67.8016   60.1618   59.2402   59.6619   60.4895  F   1    HOCN
 61.4526   62.4527   63.4488   64.4228   65.3665  F   2    HOCN
 66.2766   67.1522   67.9942   68.8041   69.5835  F   3    HOCN
 70.3343   71.0583   71.7572   72.4326   73.0858  F   4    HOCN
 73.7184   74.3314   74.9260   75.5032   76.0640  F   5    HOCN
 76.6092   77.1396   77.6560   78.1591   78.6494  F   6    HOCN
 79.1276   79.5942   80.0498   80.4948   80.9297  F   7    HOCN
 81.3549   81.7709   82.1780   82.5767   82.9673  F   8    HOCN
 83.3501   83.7255   84.0939   84.4555   84.8108  F   9    HOCN
 85.1599   85.5031   85.8409   86.1735   86.5011  F  10    HOCN
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  4.9702     4.9684     4.9676     4.9674     4.9675  CP  1   N
  4.9676     4.9676     4.9675     4.9674     4.9675  CP  2   N
  4.9689     4.9696     4.9696     4.9692     4.9684  CP  3   N
  4.9675     4.9666     4.9658     4.9653     4.9652  CP  4   N
  4.9656     4.9667     4.9686     4.9714     4.9751  CP  5   N
  4.9800     4.9861     4.9935     5.0022     5.0125  CP  6   N
  5.0243     5.0377     5.0528     5.0697     5.0884  CP  7   N
  5.1090     5.1315     5.1560     5.1825     5.2111  CP  8   N
  5.2417     5.2745     5.3094     5.3464     5.3856  CP  9   N
  5.4270     5.4705     5.5161     5.5640     5.6139  CP 10   N
 -0.9845    -0.4876     0.0092     0.5059     1.0027  H   1   N
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  3.9833     4.4802     4.9772     5.4741     5.9710  H   3   N
  6.4678     6.9645     7.4611     7.9577     8.4542  H   4   N
  8.9507     9.4473     9.9441    10.4411    10.9384  H   5   N
 11.4361    11.9344    12.4334    12.9332    13.4339  H   6   N
 13.9357    14.4388    14.9433    15.4494    15.9573  H   7   N
 16.4672    16.9792    17.4935    18.0105    18.5301  H   8   N
 19.0527    19.5785    20.1077    20.6405    21.1771  H   9   N
 21.7177    22.2625    22.8118    23.3658    23.9247  H  10   N
 41.0267    37.0639    36.6096    36.8044    37.1724  F   1   N
 37.5844    37.9975    38.3963    38.7757    39.1345  F   2   N
 39.4733    39.7934    40.0961    40.3829    40.6551  F   3   N
 40.9140    41.1607    41.3963    41.6216    41.8374  F   4   N
 42.0445    42.2436    42.4351    42.6197    42.7978  F   5   N
 42.9699    43.1363    43.2974    43.4536    43.6051  F   6   N
 43.7522    43.8952    44.0343    44.1697    44.3016  F   7   N
 44.4303    44.5558    44.6784    44.7981    44.9152  F   8   N
 45.0298    45.1420    45.2518    45.3595    45.4651  F   9   N
 45.5687    45.6704    45.7703    45.8684    45.9649  F  10   N
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|---|---|---|---|---|---|---|---|
| 6.7663 | 6.8810 | 6.9485 | 7.0068 | 7.0824 | CP | 1 | N2 |
| 7.1901 | 7.3330 | 7.5026 | 7.6787 | 7.8295 | CP | 2 | N2 |
| 7.9481 | 8.0555 | 8.1523 | 8.2395 | 8.3178 | CP | 3 | N2 |
| 8.3880 | 8.4506 | 8.5065 | 8.5563 | 8.6005 | CP | 4 | N2 |
| 8.6398 | 8.6746 | 8.7056 | 8.7331 | 8.7576 | CP | 5 | N2 |
| 8.7796 | 8.7994 | 8.8174 | 8.8338 | 8.8490 | CP | 6 | N2 |
| 8.8633 | 8.8768 | 8.8897 | 8.9022 | 8.9145 | CP | 7 | N2 |
| 8.9266 | 8.9385 | 8.9503 | 8.9620 | 8.9736 | CP | 8 | N2 |
| 8.9850 | 8.9961 | 9.0067 | 9.0168 | 9.0260 | CP | 9 | N2 |
| 9.0342 | 9.0411 | 9.0464 | 9.0498 | 9.0509 | CP | 10 | N2 |
| -1.3618 | -0.6788 | 0.0129 | 0.7106 | 1.4148 | H | 1 | N2 |
| 2.1281 | 2.8540 | 3.5956 | 4.3548 | 5.1306 | H | 2 | N2 |
| 5.9195 | 6.7198 | 7.5303 | 8.3499 | 9.1779 | H | 3 | N2 |
| 10.0132 | 10.8552 | 11.7031 | 12.5563 | 13.4142 | H | 4 | N2 |
| 14.2763 | 15.1420 | 16.0111 | 16.8830 | 17.7576 | H | 5 | N2 |
| 18.6345 | 19.5134 | 20.3943 | 21.2769 | 22.1610 | H | 6 | N2 |
| 23.0466 | 23.9336 | 24.8220 | 25.7116 | 26.6024 | H | 7 | N2 |
| 27.4945 | 28.3877 | 29.2822 | 30.1778 | 31.0746 | H | 8 | N2 |
| 31.9725 | 32.8716 | 33.7717 | 34.6729 | 35.5750 | H | 9 | N2 |
| 36.4780 | 37.3818 | 38.2862 | 39.1910 | 40.0961 | H | 10 | N2 |
| 51.8958 | 46.4013 | 45.7680 | 46.0412 | 46.5591 | F | 1 | N2 |
| 47.1421 | 47.7305 | 48.3032 | 48.8530 | 49.3783 | F | 2 | N2 |
| 49.8794 | 50.3572 | 50.8132 | 51.2488 | 51.6657 | F | 3 | N2 |
| 52.0651 | 52.4484 | 52.8167 | 53.1711 | 53.5127 | F | 4 | N2 |
| 53.8421 | 54.1604 | 54.4681 | 54.7659 | 55.0545 | F | 5 | N2 |
| 55.3343 | 55.6059 | 55.8698 | 56.1263 | 56.3759 | F | 6 | N2 |
| 56.6189 | 56.8557 | 57.0865 | 57.3116 | 57.5314 | F | 7 | N2 |
| 57.7460 | 57.9558 | 58.1608 | 58.3614 | 58.5577 | F | 8 | N2 |
| 58.7499 | 58.9382 | 59.1226 | 59.3035 | 59.4809 | F | 9 | N2 |
| 59.6549 | 59.8257 | 59.9934 | 60.1581 | 60.3199 | F | 10 | N2 |

|  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|
| 5.5004 | 7.2785 | 8.6970 | 9.8748 | 10.9016 | CP | 1 | N2H2 |
| 11.8379 | 12.7155 | 13.5368 | 14.2754 | 14.8756 | CP | 2 | N2H2 |
| 15.3566 | 15.7915 | 16.1836 | 16.5362 | 16.8524 | CP | 3 | N2H2 |
| 17.1351 | 17.3871 | 17.6113 | 17.8101 | 17.9860 | CP | 4 | N2H2 |
| 18.1413 | 18.2783 | 18.3990 | 18.5052 | 18.5989 | CP | 5 | N2H2 |
| 18.6817 | 18.7551 | 18.8206 | 18.8794 | 18.9327 | CP | 6 | N2H2 |
| 18.9815 | 19.0268 | 19.0692 | 19.1095 | 19.1481 | CP | 7 | N2H2 |
| 19.1854 | 19.2216 | 19.2570 | 19.2914 | 19.3248 | CP | 8 | N2H2 |
| 19.3568 | 19.3871 | 19.4152 | 19.4404 | 19.4618 | CP | 9 | N2H2 |
| 19.4787 | 19.4899 | 19.4943 | 19.4906 | 19.4774 | CP | 10 | N2H2 |
| -1.4277 | -0.7852 | 0.0161 | 0.9462 | 1.9860 | H | 1 | N2H2 |
| 3.1236 | 4.3517 | 5.6648 | 7.0563 | 8.5153 | H | 2 | N2H2 |
| 10.0273 | 11.5851 | 13.1842 | 14.8205 | 16.4902 | H | 3 | N2H2 |
| 18.1899 | 19.9162 | 21.6664 | 23.4376 | 25.2276 | H | 4 | N2H2 |
| 27.0341 | 28.8553 | 30.6893 | 32.5346 | 34.3899 | H | 5 | N2H2 |
| 36.2540 | 38.1259 | 40.0048 | 41.8898 | 43.7805 | H | 6 | N2H2 |
| 45.6762 | 47.5767 | 49.4815 | 51.3904 | 53.3033 | H | 7 | N2H2 |
| 55.2200 | 57.1404 | 59.0643 | 60.9917 | 62.9225 | H | 8 | N2H2 |
| 64.8566 | 66.7938 | 68.7340 | 70.6768 | 72.6219 | H | 9 | N2H2 |
| 74.5690 | 76.5175 | 78.4668 | 80.4161 | 82.3646 | H | 10 | N2H2 |
| 58.9277 | 52.9594 | 52.2093 | 52.5651 | 53.2746 | F | 1 | N2H2 |
| 54.1121 | 54.9928 | 55.8807 | 56.7595 | 57.6211 | F | 2 | N2H2 |
| 58.4615 | 59.2781 | 60.0704 | 60.8385 | 61.5830 | F | 3 | N2H2 |
| 62.3046 | 63.0044 | 63.6832 | 64.3421 | 64.9820 | F | 4 | N2H2 |
| 65.6038 | 66.2083 | 66.7964 | 67.3689 | 67.9263 | F | 5 | N2H2 |
| 68.4696 | 68.9991 | 69.5157 | 70.0199 | 70.5121 | F | 6 | N2H2 |
| 70.9929 | 71.4628 | 71.9223 | 72.3717 | 72.8115 | F | 7 | N2H2 |
| 73.2421 | 73.6638 | 74.0770 | 74.4820 | 74.8791 | F | 8 | N2H2 |
| 75.2686 | 75.6508 | 76.0260 | 76.3944 | 76.7562 | F | 9 | N2H2 |
| 77.1117 | 77.4611 | 77.8046 | 78.1423 | 78.4745 | F | 10 | N2H2 |

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 6.7566    8.1404    9.2655   10.1840   10.9386  CP  1   N20
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13.3280   13.5101   13.6715   13.8139   13.9388  CP  3   N20
14.0479   14.1428   14.2248   14.2953   14.3557  CP  4   N20
14.4071   14.4507   14.4876   14.5186   14.5449  CP  5   N20
14.5672   14.5862   14.6027   14.6173   14.6305  CP  6   N20
14.6428   14.6546   14.6662   14.6779   14.6897  CP  7   N20
14.7018   14.7143   14.7270   14.7399   14.7526  CP  8   N20
14.7650   14.7767   14.7871   14.7960   14.8025  CP  9   N20
14.8062   14.8062   14.8017   14.7918   14.7757  CP 10   N20
-1.6024   -0.8551    0.0171    0.9911    2.0485  H   1   N20
 3.1745    4.3576    5.5881    6.8575    8.1575  H   2   N20
 9.4802   10.8223   12.1816   13.5560   14.9437  H   3   N20
16.3432   17.7529   19.1713   20.5974   22.0301  H   4   N20
23.4683   24.9112   26.3582   27.8085   29.2618  H   5   N20
30.7174   32.1751   33.6345   35.0956   36.5580  H   6   N20
38.0216   39.4865   40.9526   42.4198   43.8881  H   7   N20
45.3577   46.8285   48.3006   49.7739   51.2485  H   8   N20
52.7244   54.2015   55.6797   57.1589   58.6388  H   9   N20
60.1193   61.6000   63.0804   64.5601   66.0385  H  10   N20
59.9854   53.3617   52.5503   52.9252   53.6624  F   1   N20
54.5198   55.4082   56.2907   57.1511   57.9825  F   2   N20
58.7821   59.5496   60.2856   60.9917   61.6695  F   3   N20
62.3206   62.9468   63.5497   64.1307   64.6913  F   4   N20
65.2326   65.7560   66.2624   66.7528   67.2282  F   5   N20
67.6895   68.1373   68.5724   68.9955   69.4072  F   6   N20
69.8081   70.1987   70.5795   70.9509   71.3135  F   7   N20
71.6676   72.0136   72.3519   72.6827   73.0065  F   8   N20
73.3234   73.6338   73.9380   74.2362   74.5286  F   9   N20
74.8154   75.0969   75.3732   75.6445   75.9110  F  10   N20
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  7.2202    8.5257    9.5970   10.4812   11.2167  CP  1    NCO
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 13.5470   13.7100   13.8538   13.9802   14.0906  CP  3    NCO
 14.1866   14.2696   14.3409   14.4018   14.4535  CP  4    NCO
 14.4972   14.5339   14.5646   14.5903   14.6117  CP  5    NCO
 14.6298   14.6452   14.6585   14.6704   14.6814  CP  6    NCO
 14.6918   14.7022   14.7127   14.7236   14.7351  CP  7    NCO
 14.7473   14.7602   14.7737   14.7877   14.8021  CP  8    NCO
 14.8166   14.8308   14.8444   14.8569   14.8679  CP  9    NCO
 14.8765   14.8823   14.8845   14.8822   14.8745  CP 10    NCO
 -1.6796   -0.8901    0.0177    1.0230    2.1090  H   1    NCO
  3.2624    4.4722    5.7292    7.0246    8.3494  H   2    NCO
  9.6951   11.0581   12.4365   13.8283   15.2320  H   3    NCO
 16.6460   18.0689   19.4995   20.9367   22.3795  H   4    NCO
 23.8271   25.2788   26.7337   28.1915   29.6516  H   5    NCO
 31.1137   32.5775   34.0427   35.5092   36.9768  H   6    NCO
 38.4454   39.9151   41.3859   42.8577   44.3306  H   7    NCO
 45.8047   47.2801   48.7568   50.2348   51.7143  H   8    NCO
 53.1953   54.6776   56.1614   57.6465   59.1327  H   9    NCO
 60.6200   62.1080   63.5963   65.0847   66.5726  H  10    NCO
 63.2467   56.3215   55.4781   55.8656   56.6254  F   1    NCO
 57.5073   58.4196   59.3248   60.2066   61.0579  F   2    NCO
 61.8760   62.6605   63.4123   64.1329   64.8240  F   3    NCO
 65.4874   66.1250   66.7384   67.3292   67.8988  F   4    NCO
 68.4486   68.9798   69.4935   69.9908   70.4727  F   5    NCO
 70.9400   71.3935   71.8340   72.2621   72.6786  F   6    NCO
 73.0840   73.4789   73.8638   74.2391   74.6054  F   7    NCO
 74.9631   75.3124   75.6539   75.9878   76.3145  F   8    NCO
 76.6344   76.9475   77.2544   77.5551   77.8500  F   9    NCO
 78.1392   78.4230   78.7016   78.9751   79.2438  F  10    NCO
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|---|---|---|---|---|---|---|---|
| 6.8238 | 6.9186 | 6.9599 | 6.9792 | 7.0009 | CP | 1 | NH |
| 7.0419 | 7.1115 | 7.2119 | 7.3376 | 7.4757 | CP | 2 | NH |
| 7.6092 | 7.7336 | 7.8497 | 7.9579 | 8.0589 | CP | 3 | NH |
| 8.1533 | 8.2416 | 8.3244 | 8.4021 | 8.4752 | CP | 4 | NH |
| 8.5442 | 8.6094 | 8.6714 | 8.7304 | 8.7868 | CP | 5 | NH |
| 8.8411 | 8.8933 | 8.9439 | 8.9932 | 9.0412 | CP | 6 | NH |
| 9.0884 | 9.1347 | 9.1805 | 9.2258 | 9.2707 | CP | 7 | NH |
| 9.3155 | 9.3600 | 9.4044 | 9.4487 | 9.4928 | CP | 8 | NH |
| 9.5368 | 9.5806 | 9.6241 | 9.6673 | 9.7099 | CP | 9 | NH |
| 9.7519 | 9.7930 | 9.8332 | 9.8721 | 9.9095 | CP | 10 | NH |
| -1.3691 | -0.6814 | 0.0129 | 0.7099 | 1.4088 | H | 1 | NH |
| 2.1107 | 2.8181 | 3.5341 | 4.2614 | 5.0020 | H | 2 | NH |
| 5.7563 | 6.5235 | 7.3028 | 8.0932 | 8.8941 | H | 3 | NH |
| 9.7048 | 10.5246 | 11.3529 | 12.1893 | 13.0332 | H | 4 | NH |
| 13.8842 | 14.7419 | 15.6060 | 16.4761 | 17.3520 | H | 5 | NH |
| 18.2334 | 19.1201 | 20.0120 | 20.9088 | 21.8106 | H | 6 | NH |
| 22.7171 | 23.6282 | 24.5440 | 25.4643 | 26.3891 | H | 7 | NH |
| 27.3184 | 28.2522 | 29.1904 | 30.1331 | 31.0802 | H | 8 | NH |
| 32.0316 | 32.9875 | 33.9477 | 34.9123 | 35.8812 | H | 9 | NH |
| 36.8543 | 37.8315 | 38.8128 | 39.7981 | 40.7872 | H | 10 | NH |
| 49.4499 | 43.9290 | 43.2936 | 43.5669 | 44.0835 | F | 1 | NH |
| 44.6628 | 45.2452 | 45.8093 | 46.3485 | 46.8616 | F | 2 | NH |
| 47.3494 | 47.8136 | 48.2561 | 48.6785 | 49.0824 | F | 3 | NH |
| 49.4695 | 49.8410 | 50.1982 | 50.5422 | 50.8739 | F | 4 | NH |
| 51.1941 | 51.5038 | 51.8035 | 52.0940 | 52.3758 | F | 5 | NH |
| 52.6494 | 52.9154 | 53.1741 | 53.4260 | 53.6715 | F | 6 | NH |
| 53.9108 | 54.1444 | 54.3724 | 54.5952 | 54.8130 | F | 7 | NH |
| 55.0261 | 55.2347 | 55.4389 | 55.6391 | 55.8352 | F | 8 | NH |
| 56.0276 | 56.2164 | 56.4017 | 56.5836 | 56.7624 | F | 9 | NH |
| 56.9380 | 57.1107 | 57.2806 | 57.4477 | 57.6121 | F | 10 | NH |

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|---|---|---|---|---|---|---|---|
| 7.3609 | 7.7312 | 8.0079 | 8.2510 | 8.5033 | CP | 1 | NH2 |
| 8.7905 | 9.1214 | 9.4877 | 9.8640 | 10.2079 | CP | 2 | NH2 |
| 10.5077 | 10.7892 | 11.0537 | 11.3023 | 11.5363 | CP | 3 | NH2 |
| 11.7568 | 11.9647 | 12.1611 | 12.3469 | 12.5229 | CP | 4 | NH2 |
| 12.6899 | 12.8488 | 13.0002 | 13.1447 | 13.2829 | CP | 5 | NH2 |
| 13.4153 | 13.5424 | 13.6647 | 13.7824 | 13.8958 | CP | 6 | NH2 |
| 14.0052 | 14.1108 | 14.2126 | 14.3108 | 14.4053 | CP | 7 | NH2 |
| 14.4961 | 14.5831 | 14.6661 | 14.7449 | 14.8191 | CP | 8 | NH2 |
| 14.8886 | 14.9527 | 15.0112 | 15.0635 | 15.1091 | CP | 9 | NH2 |
| 15.1472 | 15.1772 | 15.1984 | 15.2099 | 15.2110 | CP | 10 | NH2 |
| -1.5283 | -0.7726 | 0.0148 | 0.8278 | 1.6653 | H | 1 | NH2 |
| 2.5297 | 3.4249 | 4.3552 | 5.3228 | 6.3269 | H | 2 | NH2 |
| 7.3628 | 8.4278 | 9.5201 | 10.6380 | 11.7801 | H | 3 | NH2 |
| 12.9448 | 14.1310 | 15.3374 | 16.5629 | 17.8064 | H | 4 | NH2 |
| 19.0672 | 20.3442 | 21.6367 | 22.9440 | 24.2654 | H | 5 | NH2 |
| 25.6003 | 26.9483 | 28.3087 | 29.6811 | 31.0650 | H | 6 | NH2 |
| 32.4601 | 33.8659 | 35.2821 | 36.7083 | 38.1442 | H | 7 | NH2 |
| 39.5893 | 41.0433 | 42.5057 | 43.9763 | 45.4546 | H | 8 | NH2 |
| 46.9400 | 48.4321 | 49.9304 | 51.4341 | 52.9428 | H | 9 | NH2 |
| 54.4557 | 55.9720 | 57.4909 | 59.0114 | 60.5325 | H | 10 | NH2 |
| 53.4277 | 47.2308 | 46.5073 | 46.8243 | 47.4310 | F | 1 | NH2 |
| 48.1207 | 48.8234 | 49.5138 | 50.1829 | 50.8278 | F | 2 | NH2 |
| 51.4483 | 52.0451 | 52.6193 | 53.1722 | 53.7053 | F | 3 | NH2 |
| 54.2198 | 54.7170 | 55.1981 | 55.6641 | 56.1160 | F | 4 | NH2 |
| 56.5547 | 56.9810 | 57.3956 | 57.7992 | 58.1924 | F | 5 | NH2 |
| 58.5759 | 58.9500 | 59.3153 | 59.6723 | 60.0213 | F | 6 | NH2 |
| 60.3628 | 60.6970 | 61.0243 | 61.3451 | 61.6595 | F | 7 | NH2 |
| 61.9679 | 62.2705 | 62.5676 | 62.8593 | 63.1459 | F | 8 | NH2 |
| 63.4276 | 63.7044 | 63.9767 | 64.2446 | 64.5081 | F | 9 | NH2 |
| 64.7675 | 65.0229 | 65.2743 | 65.5220 | 65.7659 | F | 10 | NH2 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 6.1264 | 7.4482 | 8.4798 | 9.3303 | 10.0832 | CP | 1 | NH3 |
| 10.7968 | 11.5038 | 12.2116 | 12.9022 | 13.5321 | CP | 2 | NH3 |
| 14.0878 | 14.5994 | 15.0695 | 15.5007 | 15.8955 | CP | 3 | NH3 |
| 16.2563 | 16.5854 | 16.8850 | 17.1572 | 17.4041 | CP | 4 | NH3 |
| 17.6277 | 17.8296 | 18.0118 | 18.1758 | 18.3233 | CP | 5 | NH3 |
| 18.4556 | 18.5742 | 18.6804 | 18.7754 | 18.8602 | CP | 6 | NH3 |
| 18.9359 | 19.0034 | 19.0635 | 19.1170 | 19.1645 | CP | 7 | NH3 |
| 19.2066 | 19.2436 | 19.2761 | 19.3042 | 19.3281 | CP | 8 | NH3 |
| 19.3479 | 19.3637 | 19.3752 | 19.3824 | 19.3850 | CP | 9 | NH3 |
| 19.3825 | 19.3745 | 19.3604 | 19.3396 | 19.3114 | CP | 10 | NH3 |
| -1.4643 | -0.7827 | 0.0157 | 0.9073 | 1.8785 | H | 1 | NH3 |
| 2.9227 | 4.0377 | 5.2235 | 6.4794 | 7.8019 | H | 2 | NH3 |
| 9.1833 | 10.6180 | 12.1018 | 13.6306 | 15.2007 | H | 3 | NH3 |
| 16.8086 | 18.4509 | 20.1246 | 21.8270 | 23.5552 | H | 4 | NH3 |
| 25.3070 | 27.0801 | 28.8723 | 30.6818 | 32.5069 | H | 5 | NH3 |
| 34.3460 | 36.1976 | 38.0604 | 39.9333 | 41.8151 | H | 6 | NH3 |
| 43.7050 | 45.6020 | 47.5054 | 49.4145 | 51.3286 | H | 7 | NH3 |
| 53.2472 | 55.1698 | 57.0958 | 59.0248 | 60.9565 | H | 8 | NH3 |
| 62.8903 | 64.8259 | 66.7629 | 68.7008 | 70.6393 | H | 9 | NH3 |
| 72.5777 | 74.5156 | 76.4524 | 78.3874 | 80.3200 | H | 10 | NH3 |
| 52.8362 | 46.7785 | 46.0358 | 46.3790 | 47.0543 | F | 1 | NH3 |
| 47.8420 | 48.6624 | 49.4835 | 50.2920 | 51.0822 | F | 2 | NH3 |
| 51.8519 | 52.6000 | 53.3267 | 54.0324 | 54.7178 | F | 3 | NH3 |
| 55.3838 | 56.0313 | 56.6610 | 57.2738 | 57.8705 | F | 4 | NH3 |
| 58.4518 | 59.0184 | 59.5710 | 60.1102 | 60.6366 | F | 5 | NH3 |
| 61.1506 | 61.6529 | 62.1438 | 62.6240 | 63.0936 | F | 6 | NH3 |
| 63.5533 | 64.0033 | 64.4441 | 64.8759 | 65.2991 | F | 7 | NH3 |
| 65.7140 | 66.1209 | 66.5201 | 66.9118 | 67.2963 | F | 8 | NH3 |
| 67.6739 | 68.0446 | 68.4089 | 68.7669 | 69.1187 | F | 9 | NH3 |
| 69.4646 | 69.8047 | 70.1393 | 70.4684 | 70.7923 | F | 10 | NH3 |

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  7.3803    7.8350    8.3204    8.8307    9.3557  CP  1    HN2
  9.8805   10.3857   10.8470   11.2357   11.5186  CP  2    HN2
 11.7299   11.9280   12.1130   12.2848   12.4433  CP  3    HN2
 12.5888   12.7212   12.8410   12.9483   13.0437  CP  4    HN2
 13.1277   13.2006   13.2633   13.3164   13.3607  CP  5    HN2
 13.3971   13.4264   13.4498   13.4684   13.4832  CP  6    HN2
 13.4956   13.5069   13.5185   13.5318   13.5485  CP  7    HN2
 13.5701   13.5984   13.6352   13.6823   13.7417  CP  8    HN2
 13.8154   13.9056   14.0142   14.1437   14.2964  CP  9    HN2
 14.4746   14.6809   14.9178   15.1879   15.4940  CP 10    HN2
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  2.7439    3.7575    4.8196    5.9245    7.0632  H   2    HN2
  8.2257    9.4087   10.6109   11.8309   13.0674  H   3    HN2
 14.3191   15.5847   16.8630   18.1525   19.4522  H   4    HN2
 20.7609   22.0774   23.4007   24.7297   26.0637  H   5    HN2
 27.4016   28.7428   30.0867   31.4326   32.7803  H   6    HN2
 34.1292   35.4793   36.8306   38.1831   39.5371  H   7    HN2
 40.8930   42.2513   43.6129   44.9787   46.3498  H   8    HN2
 47.7275   49.1134   50.5093   51.9170   53.3388  H   9    HN2
 54.7771   56.2347   57.7143   59.2193   60.7531  H  10    HN2
 60.6814   54.3690   53.6247   53.9570   54.6017  F   1    HN2
 55.3448   56.1116   56.8725   57.6152   58.3342  F   2    HN2
 59.0273   59.6939   60.3344   60.9500   61.5421  F   3    HN2
 62.1120   62.6612   63.1910   63.7026   64.1970  F   4    HN2
 64.6755   65.1389   65.5881   66.0239   66.4470  F   5    HN2
 66.8581   67.2579   67.6468   68.0256   68.3945  F   6    HN2
 68.7542   69.1049   69.4472   69.7815   70.1080  F   7    HN2
 70.4271   70.7391   71.0444   71.3433   71.6360  F   8    HN2
 71.9228   72.2039   72.4797   72.7503   73.0161  F   9    HN2
 73.2772   73.5339   73.7864   74.0350   74.2798  F  10    HN2
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|  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|
| 6.9024 | 7.0198 | 7.1061 | 7.1942 | 7.3056 | CP | 1 | NO |
| 7.4501 | 7.6255 | 7.8184 | 8.0034 | 8.1435 | CP | 2 | NO |
| 8.2409 | 8.3286 | 8.4073 | 8.4778 | 8.5406 | CP | 3 | NO |
| 8.5966 | 8.6463 | 8.6904 | 8.7293 | 8.7636 | CP | 4 | NO |
| 8.7939 | 8.8207 | 8.8443 | 8.8651 | 8.8837 | CP | 5 | NO |
| 8.9003 | 8.9153 | 8.9289 | 8.9415 | 8.9533 | CP | 6 | NO |
| 8.9645 | 8.9752 | 8.9857 | 8.9960 | 9.0062 | CP | 7 | NO |
| 9.0165 | 9.0267 | 9.0370 | 9.0473 | 9.0575 | CP | 8 | NO |
| 9.0676 | 9.0774 | 9.0868 | 9.0956 | 9.1036 | CP | 9 | NO |
| 9.1105 | 9.1162 | 9.1202 | 9.1223 | 9.1221 | CP | 10 | NO |
| -1.3898 | -0.6933 | 0.0131 | 0.7280 | 1.4528 | H | 1 | NO |
| 2.1903 | 2.9438 | 3.7160 | 4.5073 | 5.3152 | H | 2 | NO |
| 6.1345 | 6.9630 | 7.7999 | 8.6442 | 9.4952 | H | 3 | NO |
| 10.3521 | 11.2143 | 12.0812 | 12.9522 | 13.8269 | H | 4 | NO |
| 14.7048 | 15.5856 | 16.4688 | 17.3543 | 18.2418 | H | 5 | NO |
| 19.1310 | 20.0218 | 20.9140 | 21.8075 | 22.7023 | H | 6 | NO |
| 23.5982 | 24.4952 | 25.3932 | 26.2923 | 27.1924 | H | 7 | NO |
| 28.0936 | 28.9957 | 29.8989 | 30.8031 | 31.7084 | H | 8 | NO |
| 32.6146 | 33.5219 | 34.4301 | 35.3392 | 36.2492 | H | 9 | NO |
| 37.1599 | 38.0713 | 38.9831 | 39.8952 | 40.8075 | H | 10 | NO |
| 56.5978 | 50.9895 | 50.3424 | 50.6222 | 51.1535 | F | 1 | NO |
| 51.7528 | 52.3590 | 52.9503 | 53.5190 | 54.0630 | F | 2 | NO |
| 54.5822 | 55.0773 | 55.5497 | 56.0009 | 56.4323 | F | 3 | NO |
| 56.8454 | 57.2415 | 57.6218 | 57.9876 | 58.3397 | F | 4 | NO |
| 58.6792 | 59.0069 | 59.3235 | 59.6297 | 59.9263 | F | 5 | NO |
| 60.2137 | 60.4924 | 60.7631 | 61.0261 | 61.2819 | F | 6 | NO |
| 61.5307 | 61.7731 | 62.0093 | 62.2395 | 62.4642 | F | 7 | NO |
| 62.6836 | 62.8978 | 63.1073 | 63.3120 | 63.5124 | F | 8 | NO |
| 63.7084 | 63.9005 | 64.0886 | 64.2729 | 64.4537 | F | 9 | NO |
| 64.6310 | 64.8050 | 64.9757 | 65.1434 | 65.3081 | F | 10 | NO |

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  6.7155     7.8712     8.8302     9.6384    10.3306  CP  1    NO2
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 12.6634    12.8155    12.9496    13.0674    13.1702  CP  3    NO2
 13.2594    13.3365    13.4026    13.4590    13.5067  CP  4    NO2
 13.5469    13.5805    13.6084    13.6316    13.6509  CP  5    NO2
 13.6668    13.6802    13.6917    13.7016    13.7106  CP  6    NO2
 13.7190    13.7272    13.7354    13.7437    13.7525  CP  7    NO2
 13.7616    13.7712    13.7811    13.7912    13.8013  CP  8    NO2
 13.8112    13.8206    13.8289    13.8358    13.8408  CP  9    NO2
 13.8432    13.8423    13.8375    13.8280    13.8128  CP 10    NO2
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  3.0039     4.1236     5.2914     6.4991     7.7370  H   2    NO2
  8.9950    10.2691    11.5575    12.8584    14.1704  H   3    NO2
 15.4920    16.8219    18.1590    19.5021    20.8505  H   4    NO2
 22.2032    23.5596    24.9191    26.2811    27.6453  H   5    NO2
 29.0112    30.3786    31.7472    33.1169    34.4875  H   6    NO2
 35.8590    37.2313    38.6044    39.9784    41.3532  H   7    NO2
 42.7289    44.1055    45.4831    46.8617    48.2414  H   8    NO2
 49.6220    51.0036    52.3861    53.7693    55.1532  H   9    NO2
 56.5374    57.9217    59.3057    60.6890    62.0711  H  10    NO2
 64.5055    58.1149    57.3382    57.6946    58.3934  F   1    NO2
 59.2050    60.0456    60.8809    61.6960    62.4843  F   2    NO2
 63.2429    63.9711    64.6695    65.3393    65.9821  F   3    NO2
 66.5994    67.1929    67.7641    68.3143    68.8449  F   4    NO2
 69.3572    69.8522    70.3311    70.7947    71.2439  F   5    NO2
 71.6796    72.1025    72.5132    72.9125    73.3010  F   6    NO2
 73.6791    74.0474    74.4064    74.7566    75.0982  F   7    NO2
 75.4319    75.7578    76.0763    76.3878    76.6926  F   8    NO2
 76.9909    77.2831    77.5693    77.8498    78.1248  F   9    NO2
 78.3946    78.6593    78.9191    79.1741    79.4246  F  10    NO2
 5.5740     5.3717     5.2313     5.1382     5.0799  CP  1    0
 5.0456     5.0264     5.0153     5.0071     4.9983  CP  2    0
 4.9942     4.9903     4.9869     4.9838     4.9812  CP  3    0
 4.9791     4.9774     4.9762     4.9755     4.9754  CP  4    0
 4.9758     4.9768     4.9783     4.9804     4.9831  CP  5    0
 4.9863     4.9902     4.9946     4.9996     5.0052  CP  6    0
 5.0114     5.0181     5.0253     5.0331     5.0414  CP  7    0
 5.0502     5.0595     5.0693     5.0794     5.0900  CP  8    0
 5.1010     5.1123     5.1239     5.1359     5.1480  CP  9    0
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 1.5446     2.0481     2.5501     3.0513     3.5515  H   2    0
 4.0512     4.5504     5.0492     5.5478     6.0460  H   3    0
 6.5440     7.0418     7.5395     8.0371     8.5346  H   4    0
 9.0322     9.5298    10.0276    10.5255    11.0237  H   5    0
11.5221    12.0209    12.5202    13.0199    13.5201  H   6    0
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19.0732    19.5838    20.0956    20.6086    21.1228  H   9    0
21.6382    22.1549    22.6728    23.1920    23.7125  H  10    0
43.2154    38.9459    38.4632    38.6671    39.0494  F   1    0
39.4749    39.8996    40.3082    40.6958    41.0617  F   2    0
41.4065    41.7318    42.0390    42.3298    42.6056  F   3    0
42.8677    43.1172    43.3553    43.5829    43.8009  F   4    0
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44.9429    45.1105    45.2728    45.4300    45.5825  F   6    0
45.7306    45.8744    46.0143    46.1504    46.2830  F   7    0
46.4122    46.5382    46.6612    46.7813    46.8987  F   8    0
47.0134    47.1256    47.2355    47.3430    47.4484  F   9    0
47.5517    47.6530    47.7523    47.8498    47.9455  F  10    0
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  6.5991     6.8045     7.0096     7.2197     7.4358  CP  1    02
  7.6546     7.8690     8.0674     8.2340     8.3490  CP  2    02
  8.4290     8.5060     8.5802     8.6516     8.7205  CP  3    02
  8.7869     8.8511     8.9130     8.9729     9.0308  CP  4    02
  9.0868     9.1411     9.1937     9.2448     9.2944  CP  5    02
  9.3426     9.3894     9.4350     9.4794     9.5226  CP  6    02
  9.5648     9.6058     9.6459     9.6851     9.7232  CP  7    02
  9.7605     9.7969     9.8324     9.8670     9.9007  CP  8    02
  9.9336     9.9656     9.9967    10.0269    10.0562  CP  9    02
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 10.5757    11.4576    12.3458    13.2401    14.1403  H   4    02
 15.0462    15.9576    16.8744    17.7963    18.7233  H   5    02
 19.6551    20.5918    21.5330    22.4787    23.4288  H   6    02
 24.3832    25.3417    26.3043    27.2709    28.2413  H   7    02
 29.2155    30.1934    31.1749    32.1598    33.1482  H   8    02
 34.1400    35.1349    36.1330    37.1342    38.1384  H   9    02
 39.1454    40.1553    41.1677    42.1828    43.2003  H  10    02
 55.0894    49.6361    49.0019    49.2794    49.8103  F   1    02
 50.4135    51.0273    51.6285    52.2084    52.7640  F   2    02
 53.2945    53.8005    54.2832    54.7442    55.1849  F   3    02
 55.6069    56.0116    56.4002    56.7741    57.1341  F   4    02
 57.4814    57.8168    58.1410    58.4550    58.7592  F   5    02
 59.0543    59.3409    59.6194    59.8903    60.1541  F   6    02
 60.4111    60.6617    60.9062    61.1449    61.3781  F   7    02
 61.6060    61.8290    62.0472    62.2608    62.4701  F   8    02
 62.6753    62.8764    63.0737    63.2673    63.4573  F   9    02
 63.6440    63.8274    64.0076    64.1848    64.3590  F  10    02
 7.2353    7.2028    7.1523    7.1022    7.0667  CP  1    HO
 7.0564    7.0775    7.1323    7.2192    7.3325  CP  2    HO
 7.4528    7.5668    7.6746    7.7766    7.8729  CP  3    HO
 7.9637    8.0494    8.1301    8.2059    8.2772  CP  4    HO
 8.3442    8.4070    8.4659    8.5211    8.5727  CP  5    HO
 8.6210    8.6661    8.7084    8.7478    8.7847  CP  6    HO
 8.8193    8.8516    8.8820    8.9105    8.9374  CP  7    HO
 8.9628    8.9869    9.0099    9.0319    9.0531  CP  8    HO
 9.0737    9.0939    9.1137    9.1333    9.1529  CP  9    HO
 9.1727    9.1928    9.2133    9.2344    9.2562  CP 10    HO
-1.4267   -0.7046    0.0132    0.7259    1.4342  H   1    HO
 2.1401    2.8465    3.5567    4.2740    5.0014  H   2    HO
 5.7407    6.4918    7.2539    8.0265    8.8090  H   3    HO
 9.6009   10.4016   11.2106   12.0275   12.8517  H   4    HO
13.6828   14.5204   15.3640   16.2134   17.0681  H   5    HO
17.9278   18.7922   19.6610   20.5338   21.4104  H   6    HO
22.2907   23.1742   24.0609   24.9506   25.8430  H   7    HO
26.7380   27.6355   28.5353   29.4374   30.3417  H   8    HO
31.2481   32.1564   33.0668   33.9792   34.8935  H   9    HO
35.8098   36.7280   37.6483   38.5707   39.4952  H  10    HO
50.2718   44.5342   43.8783   44.1583   44.6853  F   1    HO
45.2739   45.8632   46.4320   46.9737   47.4875  F   2    HO
47.9746   48.4371   48.8769   49.2961   49.6965  F   3    HO
50.0797   50.4470   50.7999   51.1394   51.4666  F   4    HO
51.7823   52.0874   52.3825   52.6684   52.9457  F   5    HO
53.2148   53.4762   53.7305   53.9779   54.2189  F   6    HO
54.4538   54.6829   54.9065   55.1249   55.3383  F   7    HO
55.5469   55.7510   55.9507   56.1463   56.3378  F   8    HO
56.5256   56.7097   56.8902   57.0674   57.2413  F   9    HO
57.4120   57.5798   57.7446   57.9066   58.0659  F  10    HO
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